

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204 Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.					
1. AGENCY USE ONLY (Leave Blank)		2. REPORT DATE 07/12/99		3. REPORT TYPE AND DATES COVERED Final Report October 1997- December 1998	
4. TITLE AND SUBTITLE Simulation of dislocation and transformation plasticity in shape memory alloys.				5. FUNDING NUMBERS N 68171-97-M-5779	
6. AUTHOR(S) Alexander E. Volkov					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Research Inst. of Mathematics and Mechanics (NIIMM) of the St.-Petersburg State Univ. Bibliotechnaya pl., 2, Petrodvorets, 198904 St.-Petersburg, Russia				8. PERFORMING ORGANIZATION REPORT NUMBER Final Report	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) European Research Office of the U.S. Army. USARDSG-UK Edison House, 223 Old Marylebone Road, London, NW1 5TH United Kingdom.				10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES					
12a. DISTRIBUTION/AVAILABILITY STATEMENT DISTRIBUTION STATEMENT A Approved for Public Release Distribution Unlimited				12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) A model of deformation of shape memory alloys has been developed. It takes into account deformation due to the phase transformation and plastic deformation, produced by an external stress or by inter-phase stresses (micro-plastic deformation at accommodation of martensite). Constitutive equations are formulated basing on the background general microstructural approach named structure-analytical theory of strength. Equations describing variation of martensite content, phase and plastic deformations are formulated on the micro-level with the account of the symmetry and kinetics of these processes, appearance of internal stresses. Macroscopic quantities are obtained by averaging. Two variants of the model have been developed for alloys of Ti-Ni and Fe-Mn-Si types. Stress-strain and strain-temperature dependencies including strain accumulation at thermal cycling and two-way shape memory effect have been described. An account of inter-grain stresses allowed to model some finer effects. A series of experiments has been carried out to study the influence of active plastic deformation on shape memory effects in TiNi alloys.					
14. SUBJECT ITEMS shape memory alloys, thermocycling, modelling, plastic deformation				15. NUMBER OF PAGES	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT		

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

AD

**SIMULATION OF DISLOCATION AND TRANSFORMATION
PLASTICITY IN SHAPE MEMORY ALLOYS**

Final Technical Report
by
Volkov A.E., Evard M.E.
(July 1999)

United States Army

EUROPEAN RESEARCH OFFICE OF THE U.S. ARMY
London, England

CONTRACT NUMBER N 68171-97-M-5779

R+O no: 8174-AN-01.

Research Institute of Mathematics and Mechanics (NIIMM)
of the St.-Petersburg State University
Bibliotechnaya pl., 2, Petrodvorets, 198904, St.-Petersburg, RUSSIA

Approved for Public Release; distribution unlimited

19991004 056

SIMULATION OF DISLOCATION AND TRANSFORMATION PLASTICITY IN SHAPE MEMORY ALLOYS

Summary of results

There has been developed a model of deformation of shape memory alloys based on the methodology of the background microstructural approach proposed by Prof. V.A.Likhachev and named the structure-analytical theory of strength. Two scales of plastic deformation are modeled. The first is the micro-plastic deformation caused by the interphase stresses arising at the accommodation of martensite; the second is the active plastic deformation, produced by external mechanical loading. Constitutive equations for alloys of TiNi- and FeMnSi-types have been formulated and computer programs composed. The model can describe such phenomena as the incompleteness of the strain recovery at thermocycles, plastic deformation of austenite, repeated two-way shape memory effect, produced both by micro-plastic and macro-plastic deformation. Calculated dependencies are in a good qualitative agreement with the available experimental data.

Publications

The results obtained within the frames of the project have been published in the following works.

[1*] Evard M.E., Volkov A. E. Modeling of strain accumulation and recovery due to fcc-hcp transformation at thermocycles // Preprints of 2nd Int. workshop on new approaches to hi-tech materials (8 – 12 June 1998, St.Petersburg). St.Petersburg, 1998. F3. (The full text of the article is published in Proceedings of SPIE)

[2*] Miller D., Lagoudas D., Evard M.E., Volkov A. E. Influence of plastic strain on the shape memory effect of NiTi wires // Proceedings of Plasticity 99: The Seventh International Symposium on Plasticity and its Current Applications, edited by Akhtar S. Khan, 1998, pp. 247-250.

[3*] Evard M.E., Volkov A. E. Modeling of martensite accommodation effect on mechanical behavior of shape memory alloys // J. Engr. Mater. and Technology. 1999, Vol. 121, N 1. P. 102 – 104.

[4*] Evard M.E., Volkov A. E. A theoretical study of the plastic deformation in titanium-nickel shape memory alloy // Proceedings of the international symposium: Shape Memory Alloys: Fundamentals, Modeling and Industrial Applications, edited by F. Trochu, V. Brailovski, A. Galibos, 1999, pp. 177 – 183.

Introduction.

At present the problem of modelling of the mechanical behaviour of shape memory alloys (SMAs) becomes more and more significant because many new applications in various fields of technology and medicine [1,3] are being developed. A computer simulation helps to check the workability of a device, optimize its parameters. In 1980s – 1990s there were developed many theoretical approaches which can describe the mechanical behaviour of SMAs. They may be divided into two groups. The first consists of phenomenological macroscopic theories [4–8] which establish a relation between stress, strain, internal

parameters and their rates mainly on the grounds of observations of their mechanical behaviour. The advantages of such theories are their compactness, a comparatively easy procedure of determining of the material constants, relatively small amounts of computation. The shortcoming is their inter- or extra- polation character, less predictive ability. The other group is formed by microstructural theories [9–12]. They are based on crystallographic and physical data about the structure of the material and mechanisms of deformation and take into account geometrical and physical peculiarities of deformation mechanisms. This allows to develop rheological models invariant of the external loading, to make predictions about the behaviour of a particular alloy under the action of a complex thermomechanical load most accurately and physically grounded. At the same time in such theories it is more difficult to calibrate material constants, big computation resources are required and this impedes their use for solving boundary-value problems. Still the necessity to describe different regimes of an SMA application in the frames of one general physically justified approach makes the use of micro-structural theories very attractive. In the present project a background microstructural approach developed by V.A.Likhachev and named "structure-analytical theory of strength" is used as the guideline and an attempt is made of its expansion to loadings causing irreversible plastic deformations.

Basic constitutive equations of structure-analytical theory of strength

The structure-analytical theory of strength [9,10] assumes that the main characteristic of a crystal, determining many of its properties and particularly deformation mechanisms, is the crystallographic orientation to which the orientation of slip systems is related. A polycrystal consists of grains differing by such orientations, therefore to obtain macro deformation it is reasonable to use orientation averaging of deformations of grains. This averaging may be supplemented with the statistical one on such parameters as the width of thermomechanical hysteresis. The averaging procedure is organized in a way to reflect the grain structure of the material [13]. In each of $1, 2, \dots, \omega, \dots, \Omega$ grains of the representative volume of a polycrystalline body the deformation related to the crystallographic basis of that grain is characterized by a matrix $\varepsilon^{Gr}(\omega)$. The macroscopic phase strain ε^M is obtained by reducing matrices $\varepsilon^{Gr}(\omega)$ to the laboratory basis and averaging on all grains:

$$\varepsilon^M = \sum_{\omega=1}^{\Omega} f(\omega) R_{\omega} \varepsilon^{Gr}(\omega) R_{\omega}^{-1}, \quad (1)$$

where R_{ω} is the rotation matrix transforming the laboratory basis into the basis of grain ω and $f(\omega)$ is the volume fraction of this grain. The volume fraction Φ^M of martensite in a grain is calculated by the same averaging procedure:

$$\Phi^M = \sum_{\omega=1}^{\Omega} f(\omega) \Phi^{Gr}(\omega), \quad (2)$$

On the total in each grain there can exist $1, \dots, n, \dots, N$ variants of martensite. A variant is characterised by quantity Φ_n , such that $(1/N)\Phi_n$ is its volume fraction in the grain, and lattice deformation D_n by which it was obtained from the parent phase. If the matrix D for one of the variants is known, the corresponding matrices D_n for other variants can be found by rotating D by operators P_n belonging to the cube symmetry group:

$$D_n = P_n D P_n^{-1}, \quad n = 1, \dots, N. \quad (3)$$

In each grain the average phase strain ε^{Ph} accumulated due to lattice deformation in the course of the transformation related to the crystallographic basis and the volume fraction of martensite are equal to

$$\varepsilon^{Ph} = \frac{1}{N} \sum_{n=1}^N \Phi_n D_n, \quad (4)$$

$$\Phi^{Gr} = \frac{1}{N} \sum_{n=1}^N \Phi_n, \quad (5)$$

For simplicity Φ^{Gr} , Φ_n , ε^{Ph} , etc. here and further are written instead of $\Phi^{Gr}(\omega)$, $\Phi_n(\omega)$, $\varepsilon^{Ph}(\omega)$, etc.

To formulate the law of variation of Φ_n we consider the thermodynamic equilibrium of the two-phase austenite-martensite system. We introduce the thermodynamic force F_n^t which is the difference of specific Gibbs energies of the n -th variant of martensite and austenite. An approximate expression for F_n^t is

$$F_n^t = (T_n^* - T_0) \cdot (q_0/T_0), \text{ with } T_n^* = T + (T_0/q_0) \tau \cdot D_n, \quad (6)$$

where T_n^* is the effective temperature, T_0 is the temperature of the equilibrium of the two phases when there is no stress, q_0 is the latent heat ($q_0 < 0$), τ is the stress and double dot sign denotes the double contraction of tensors. It is generally assumed that a moving interface overcomes a resistance, due to the energy of martensite crystal nucleation and other barriers. Here we call it friction force F^{fr} and assume that it has a constant absolute value and opposes the movement of a phase boundary. Besides friction, there appears a counter-force F_n due to the interaction between martensite crystals and austenite matrix. We postulate as the first approximation that this force can be calculated as:

$$F_n = \mu_m \Phi_n \quad (7)$$

where μ_m is a constant.

At the thermodynamic equilibrium there is the balance of forces:

$$F_n^t = F_n \pm F^{fr}, \quad (8)$$

where plus sign must be taken for the direct and minus — for the reverse transformation. Constants F^{fr} and μ_m can be determined from the kinetics of the martensitic transformation when no stress is applied and they are: $F^{fr} = (-q_0) \cdot (A_f - M_s) / (A_f + M_s)$, $\mu_m = (-q_0) \cdot 2(M_s - M_f) / (A_f + M_s)$, M_f , M_s , A_s , A_f being as usual the characteristic temperatures of the transformation. From (7) and (8) differential $d\Phi_n$ can easily be found:

$$d\Phi_n = dF_n^t / \mu_m. \quad (9)$$

Initial conditions are based on the fact that at temperatures above A_f and in stress-free state no micro deformations have begun and for all martensite variants we have $\Phi_n = 0$.

Theoretical studies of different variants of the structure-analytical model [11,13] has shown the capability of this approach to correctly describe the basic features of SMA behaviour at different regimes of thermal and mechanical loading.

Modelling of martensite accomodation effect on mechanical behavior of TiNi type shape memory alloys [3*]

The first step to expand the field of applicability of the model was to take into account micro plastic deformation and stress produced by the accommodation of martensite [14] which plays a big role in the peculiarities of SMA deformation. In particular, it has been shown that accomodation processes are connected with such phenomena as the decrease of the phase yield limit at cyclic loading [15]. They are also responsible for such phenomena as incomplete recovery of strain, strain accumulation at thermocycling and repeated two-way shape memory effect.

To describe the deformation produced by the accommodation of martensite consider equation (4) as a decomposition of the strain ε^g relative to some generalized basis $\{D_n\}$ with components Φ_n and which we therefore shall interpret as the measures of strain. As the micro plastic strain ε^{mp} caused by the accommodation of martensite is connected with the same martensite crystals as the phase strain, we postulate that ε^{mp} can be expressed in the form similar to (4).

$$\varepsilon^{mp} = \frac{1}{N} \sum_{n=1}^N \Phi_n^p D_n \quad (10)$$

where Φ_n^p is the measure of the micro plastic strain produced at the accommodation of crystals, belonging to the n -th variant of martensite in a given grain.

As the accommodation leads to a partial relaxation of interphase stresses, we assume that the resistance force F_n decreases by the quantity $\alpha_m \Phi_n^p$ (in [14] it was taken $\mu_m = \alpha_m$). So we must change equation (7) for resistance force to

$$F_n = \mu_m \Phi_n - \alpha_m F_n^p \quad (11)$$

We note that after (11) has been accepted instead of (7), formula μ_m given above is no more valid as the kinetics of the transformation is different when martensite accomodation takes place.

The evolution equation for Φ_n^p is obtained from a hypothesis that differentials $d\Phi_n^p$ and dF_n are related in the same way as the differentials of strain and stress in the classical flow theory with linear hardening. Then one can easily show that when the force F_n exceeds some yield limit F_n^y

$$d\Phi_n^p = k d\Phi_n H(|F_n| - F_n^y) H(dF_n \text{sign} F_n), \quad (12)$$

where H is the function of Heaviside, k is the coefficient characterising hardening. If $k = 0$ there is no micro plasticity, if $k \rightarrow 1$ there is ideal micro plasticity without hardening. As the counter-force F_n grows (decreases) only at the growth (decrease) of martensite, which in its

turn can occur only at the growth (decay) of the thermodynamic force F_n^t , we have $\text{sign}(dF_n) = \text{sign}(dF_n^t)$ and $H(dF_n \text{sign} F_n) = H(dF_n^t \text{sign} F_n)$. Then

$$d\Phi_n = dF_n^t / \{ \mu_m [1 - kH(|F_n| - F_n^y)H(dF_n^t \text{sign} F_n)] \} \quad (13)$$

When micro plastic deformation is in progress, the yield limit grows at the same rate as the force F_n^t whose increment is equal to that of the thermodynamic force.

Initial conditions are based on the fact that at temperatures above A_f and in stress-free state no micro deformations have begun and for all martensite variants we have $F_n^y = F_0^y = \text{const}$, $\Phi_n^p = \Phi_n = 0$.

When micro plasticity is taken into account, the strain in a grain is calculated as

$$\varepsilon^{gr} = \varepsilon^{ph} + \varepsilon^{mp} = \frac{1}{N} \sum_{n=1}^N D_n (\Phi_n + \Phi_n^p), \quad (12)$$

and the total macro strain is delivered by averaging (1). For numerical calculations the relations given above can be reduced to a system of $2N$ ordinary differential equations.

Examples of modelling

Deformation simulation was carried out for an object consisting of 120 grains of different pseudo-random orientations. The following values of material constants have been used: $M_f = 280$ K, $M_s = 300$ K, $A_s = 340$ K, $A_f = 360$ K, $T_0 = 330$ K, $q_0 = -150$ MJ/m³. The value $F_0^y = 13$ MPa has been chosen in such a way that microplasticity could take place at cooling of specimen stressed by 30 MPa. Parameter k has been varied. Calculations have been performed for cases of pure shear and uniaxial tension. Heat expansion has not been taken into account. Microplastic deformation at accommodation of martensite strongly influences mechanical behavior of shape memory alloys and especially at cyclic variations of temperature or stress. Because of this we have chosen to model strain accumulation and recovery by a specimen loaded with a constant stress of 100 MPa and subjected to temperature cycles through the full interval of the phase transformation. Fig.1 presents the kinetics of this process for $k = 0.4$. Maximum strain saturates, strain unrecovered in a cycle decreases and the hysteresis loop stabilizes in approximately 20 cycles (Fig.2).

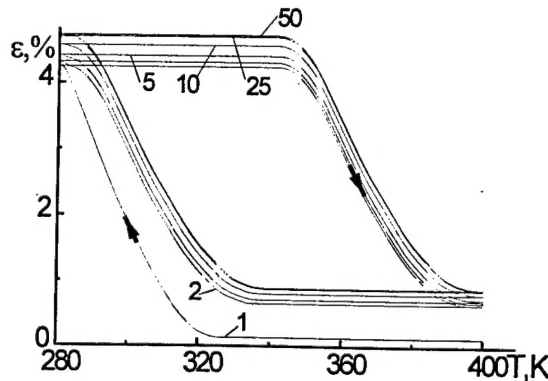


Fig.1 Strain vs. temperature dependence at thermocycling in the full interval of the martensitic transformation under the stress of 100 MPa. Numerals on the plot indicate numbers of cycles.

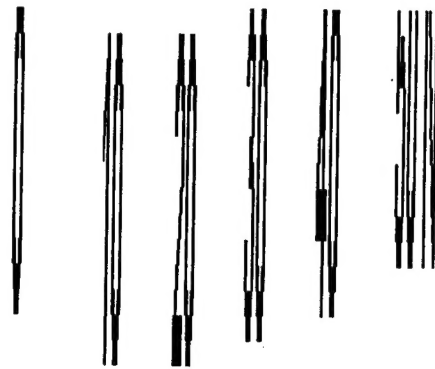
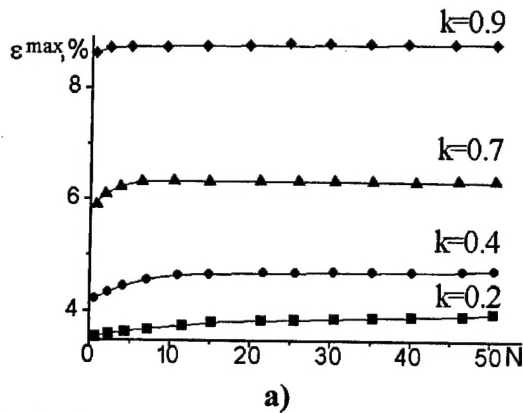


Fig.2. Calculated strain at a temperature below M_f (a) and the unreciprocity of the strain (b) in an N -th cycle. Thermal cycling was carried out through the full interval of the martensitic transformation under the stress of 100 MPa symbols in fig.2b correspond to the values of k , given in fig.2a.

An important place in the studies of the work ability of SMAs is occupied by the following thermomechanical cycle: cooling of a sample from austenite to martensite under some load P , application of an additional load Q , heating to a temperature higher than A_f and removing the additional load Q to have the initial load P . Figures 3, 4 show the result of such numerical experiment when $P = 100$ MPa, $Q = 200$ MPa. Stabilization of the loop in this case is also achieved in about 20 cycles. Strain unrecovered in a cycle becomes small and almost constant. The maximum strain accumulated up to the N -th cycle slowly grows. these results are in a good agreement with the data of the direct experiment [21]. An application of an additional load Q at a low temperature causes no unelastic strain as the stress produced by $P+Q$ is insufficient for the reorientation of martensite. As the temperature rises, the reorientation limit stress decreases. At some temperature lower than A_f the reorientation of martensite starts. Then a typical "hump" appears on the strain recovery curves in fig.3.

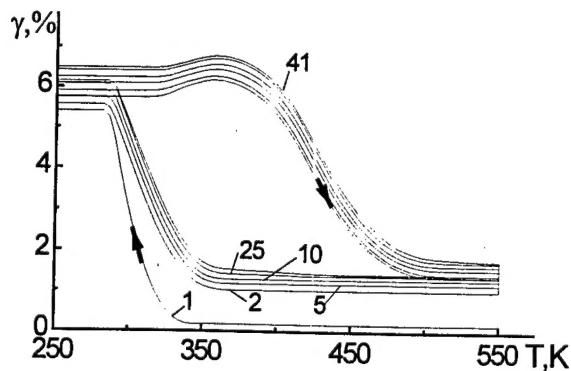


Fig. 3. Calculated strain versus temperature diagram at thermocycles with cooling under the stress 100 MPa and heating under 300 MPa (torsion). Numerals indicate numbers of cycles.

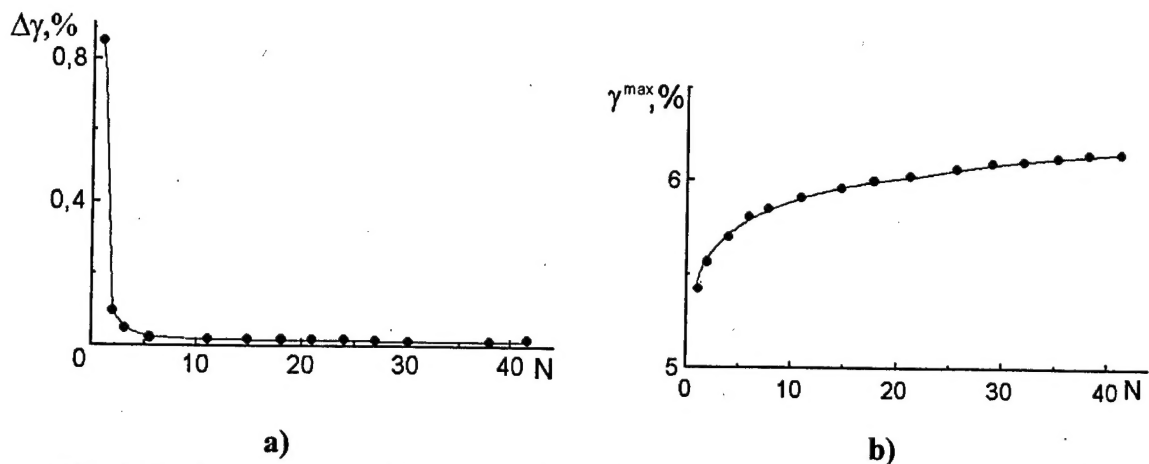


Fig. 4. Strain unrecovery (a) and maximum strain (b) as function of the number of thermocycles depicted in fig. 3.

One of the properties of SMAs which until now could not be satisfactorily described in the scheme of the structure-analytical model is the repeated two-way shape memory formed by cooling under a stress or by active straining in martensite..

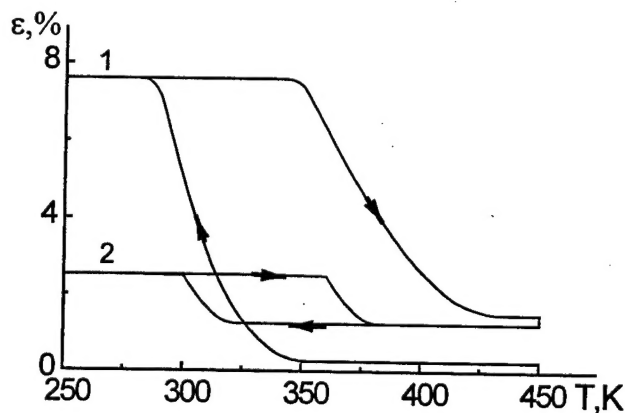


Fig. 5. Calculated strain versus temperature diagram at cooling and heating under 100 MPa (curve 1), unloading and a stress-free thermocycle (curve 2).

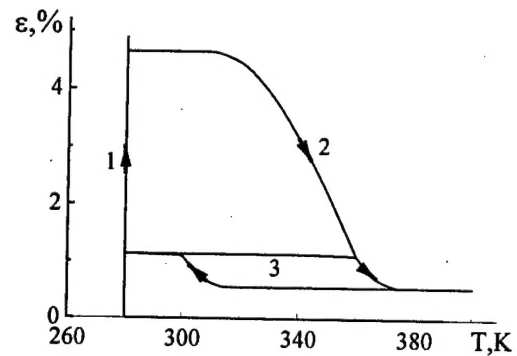


Fig. 6. Strain versus temperature diagram of active deformation of a sample in martensite state and unloading (curve 1), heating (curve 2) and subsequent stress-free thermocycle (curve 3).

The mechanism of this phenomena may lie in the appearance of micro stress fields as the result of the incompatible plastic strain accompanying the growth of martensite crystals. Figures 5 and 6 present the results of modelling of this effect. The model demonstrates a reversible strain variation which corresponds to experimental data [16]. According to existing notions [17] plastic deformation at martensite accommodation plays an important role in training of the material by thermocycling under a load, fatigue damages, the formation of eigenstresses responsible for the adaptation of the material and formation of the repeated two-way shape memory. The last thesis is confirmed by the fact that the repeated shape memory

appears only after a strong enough straining of the object by a load exceeding a critical level when there is no complete strain recovery. At the same time all these considerations were mostly pure qualitative and did not allow a passage to engineering calculations. The proposed model sets a formal ground for such notions and the agreement of calculated results with experimental ones confirms the validity of this approach. As the result it becomes possible to model thermocyclic training and repeated two-way shape memory. Calibration of the material constants allows to obtain valid results for specific alloys.

Modelling of shape memory alloys with fcc-hcp transformation (of FeMnSi type) [1*]

One of the specific features of fcc \leftrightarrow hcp transformations is the multi-variance of both direct and reverse transformations [16,18]. The result of it is that specimens loaded by a constant stress experience deformation when they undergo either of the transformations. Thus, considerable strain can be accumulated at thermal cycles. Large part of this strain is reversible and can be recovered at further cycles after the stress is removed [19]. This fact suggests that the strain is due to transformations rather than to dislocation movement. Strain accumulation at thermocycles can be described by the structure-analytical theory of strength which is distinguished by two ideas: (1) the existence of limits of the size of growing martensite crystals and (2) the possibility that the deformation of a martensite crystal at the reverse transformation is not, in general, opposite to the deformation which this crystal has undergone at the direct transformation. The model based on only these two features predicts absolutely symmetrical behaviour of a loaded sample in heating and in cooling. An attempt to account for an asymmetry has been made in [20]. However, approaches [10,20] did not take into account microplastic strain arising at the growth of martensite crystals and leading to a partial accommodation of martensite and relaxation of interphase stresses. Because of this drawback the stabilization of the deformation of the model material occurs in 3 – 5 cycles rather than in several dozens as in an actual experiment. Strain recovery at thermal cycles without stress can not be described either. The present work accounts both for symmetrical features of fcc \leftrightarrow hcp transformations and microplastic deformation.

At fcc \rightarrow hcp transformation one of $\{111\}_{\text{fcc}}$ planes becomes $(0001)_{\text{hcp}}$ by one of three shears $1/6 \langle 11\bar{2} \rangle_{\text{fcc}}$ on each second plane making up $N=12$ variants of transformation strain tensor D_n and martensite quantities Φ_n . At the reverse transformation each of three shears

$1/3 \langle 11\bar{2}0 \rangle_{\text{hcp}}$ restores the initial orientation of austenite. Thus all variants can be divided into four triplets (zones) with parameters

$$\Phi_z = \frac{1}{3} \sum_{n=3z-2}^{3z} \Phi_n, \quad z = 1, 2, 3, 4, \quad (3)$$

characterising the amount of martensite belonging to a zone, $(1/4)\Phi_z$ being the volume fraction of martensite of this zone. Parameters Φ_n themselves do not have physical meaning of martensite amounts as deformations D_n belonging to one zone produce martensite of the same orientation. Still Φ_n play the role of measures of the phase deformation. Total deformation of a grain caused by transformation and accommodation of martensite is presented by the same formula (12). Evolution equations for Φ_n is obtained by the same

considerations as for TiNi type alloys. The difference is that two extra conditions of transformation finish exist: direct transformation can not occur to make the volume fraction of martensite in a grain $\Phi^{gr} > 1$; martensite fraction in a zone (1/4) Φ_z can not become less than zero. Summarizing all this we arrive at a final form of the evolution equation:

$$d\Phi_n = \left\{ \frac{G_m + g_m}{G_m g_m} \left[H(|F_n| - F_n^y) H(-dF_n^t \text{sign} F_n) + H(F_n^y - |F_n|) \right] dF_n + \right. \\ \left. + \frac{G_m + h_m}{G_m h_m} H(|F_n| - F_n^y) H(dF_n^t \text{sign} F_n) dF_n \right\} H(1 - \Phi^{gr}) H(\Phi_z), \quad (11)$$

For numerical simulations the initial value of the yield limit ($F_0^y = 10$ MPa) was chosen such that microplasticity in cooling (and subsequent unrecovered strain in heating) took place when the stress was as small as 10 MPa. The value of the microplasticity module h_m was varied. Fig.7 presents the calculated by this model (for $h_m = 2$ MPa) diagram of strain evolution at thermal cycles. By adjusting of module h_m one can obtain different rates of thermocyclic strain production (fig.8). Simulations have also shown a decrease of M_s temperature.

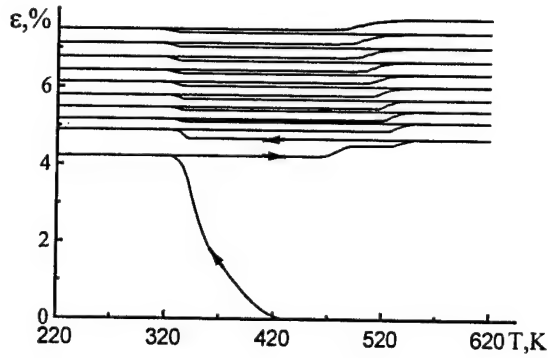


Fig. 7. Strain dependence on temperature at thermal cycles in the range 220 - 620 K under a constant stress of 50 MPa (calculation).

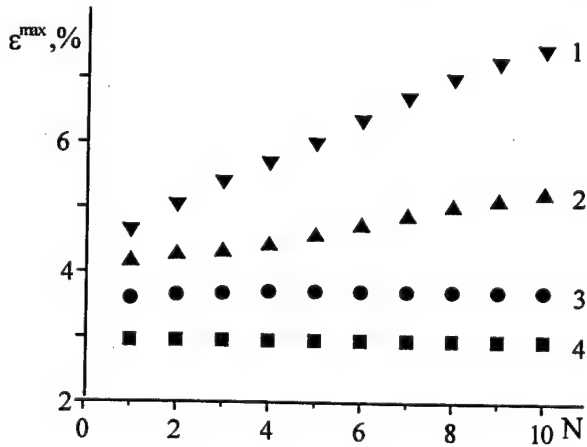


Fig.8. Maximum strain accumulated by a model sample in N thermal cycles under stress 50 MPa for different values of module h_m : 2 (1), 5 (2), 7 (3), 65 (4) MPa.

Appearance of microplastic strain gives rise to some internal stress which is obviously the cause of the experimentally observed [21] partial strain recovery at subsequent thermal cycles in an unloaded specimen. Some confirmation to this statement is supplied by the result of modelling shown in fig.9. Being very intensive for some first cycles, the recovery in a cycle then decreases. In previous works this effect was not possible to describe by means of the structure-analytical model.

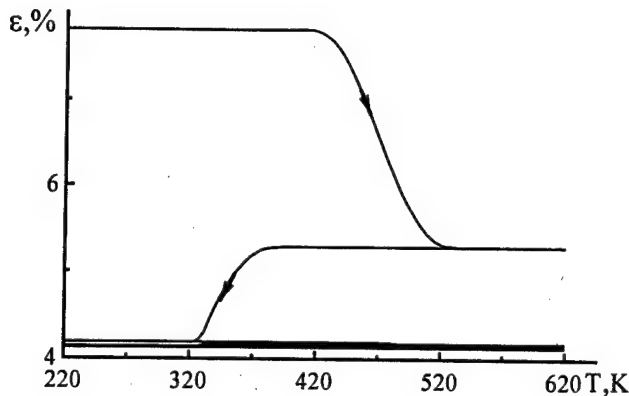


Fig.9. Strain dependence on temperature at thermal cycles without stress after preliminary treatment shown in fig. 7.

In conclusion we may state that a satisfactory simulation of the cyclic mechanical behavior of alloys with $\text{fcc} \leftrightarrow \text{hcp}$ transformations is possible only with an account of the accommodation of martensite and microplastic deformation.

Modelling of active plastic deformation in Titanium-nickel shape memory alloy [4*]

In many applications there may occur loading which causes an active plastic deformation. Besides, plastic deformation influences the quantitative characteristics and kinetics of martensitic non-elasticity giving way to the formation of such specific effects as the two-way shape memory and training of the material at cyclic temperature variations [16,21,22]. Preliminary thermomechanical treatment allows to change purposefully the functional-mechanical properties of SMA. That is why big attention is paid to the development of models allowing to calculate plastic deformation and predict its influence. Several works are devoted to the calculation of the dislocation plasticity arising at the growth of martensite crystals inside the austenitic matrix. The principles of the calculation of the plastic deformation due to dislocation slip have been formulated in the book [9]. In the present work it is developed a model of the plastic deformation of a polycrystalline TiNi specimen using the general ideas of this book.

The mathematical object is an austenitic polycrystal consisting of grains numbered $1, 2, \dots, \omega, \dots, \Omega$, each grain having several slip systems. Any slip plane may be referred to one of $1, 2, \dots, m, \dots, M$ types and $1, 2, \dots, k, \dots, K_m$ crystallographically equivalent planes belong to each type. These planes may be obtained from one of them by rotations belonging to the point symmetry group of cubic lattice.

Athermal plastic deformation $\varepsilon_{\omega}^{gr a}$ in a grain is the sum of the deformations on each of the slip planes in this grain:

$$\dot{\epsilon}_{\omega}^{gra} = \sum_{m=1}^M \sum_{k=1}^{K_m} \dot{\epsilon}_{\omega}^{a(m,k)}, \quad (1)$$

where $\epsilon_{\omega}^{a(m,k)}$ is the referred to the laboratory basis athermal deformation produced by slip on the k -th plane of the m -th type.

Let σ^{gr} be the effective stress applied to a grain. Then the stress acting on the plane (m, k) has shear components which may be written as:

$$\tau_{31}^{(m,k)} = A_{p3}^{(m,k)} A_{q1}^{(m,k)} \sigma_{pq}^{gr}, \quad \tau_{32}^{(m,k)} = A_{p3}^{(m,k)} A_{q2}^{(m,k)} \sigma_{pq}^{gr}, \quad (2)$$

where A_{pq} is the rotation matrix transferring the crystallographic basis of the grain ω into the crystallographic basis of the (m, k) plane. We assume that dislocation slip starts when the intensity of the tangential stress on the slip plane

$$T_{\tau}^{(m,k)} = \sqrt{\frac{1}{2}((\tau_{31}^{(m,k)})^2 + (\tau_{32}^{(m,k)})^2)} \quad (3)$$

reaches its critical value $\tau^{s(m,k)}$:

$$T_{\tau}^{(m,k)} = \tau^{s(m,k)}. \quad (4)$$

Due to the tangential stress

$$\tau_{\lambda\mu}^{(m,k)} = \tau_{31}^{(m,k)} (\delta_{\lambda 1} \delta_{\mu 3} + \delta_{\lambda 3} \delta_{\mu 1}) + \tau_{32}^{(m,k)} (\delta_{\lambda 2} \delta_{\mu 3} + \delta_{\lambda 3} \delta_{\mu 2}) \quad (5)$$

a shear strain is produced, having the components

$$\dot{\beta}_{31}^{a(m,k)} = \frac{1}{2} \dot{\Gamma}_{\beta}^{(m,k)} \frac{\tau_{31}}{T_{\tau}}, \quad \dot{\beta}_{32}^{a(m,k)} = \frac{1}{2} \dot{\Gamma}_{\beta}^{(m,k)} \frac{\tau_{32}}{T_{\tau}}, \quad (6)$$

where $\dot{\Gamma}_{\beta}^{(m,k)} = \sqrt{2\dot{\beta}_{pq}^{a(m,k)}\dot{\beta}_{pq}^{a(m,k)}}$ is the intensity of the shear strain rate tensor on the plane (m, k) .

We assume that the flow stress $\tau^{s(m,k)}$ is the sum of an equilibrium value $\tau^{s(m)eq}$, which is the same for all planes of the given m -th type, and additions responsible for the deformation $\tau^{s(m,k)def}$ and latent hardening:

$$\tau^{s(m,k)} = \tau^{s(m,k)eq} + \tau^{s(m,k)def} + C_{\tau} \sum_{m,k} \tau^{s(m,k)def}, \quad (7)$$

where C_{τ} is an empirical constant and the last term is due to the latent hardening connected with the possibility of simultaneous plastic deformation on several slip planes. This formula does not take into account the strain rate dependence of the flow stress.

The component $\tau^{s(m,k)eq}$ we shall write as follows:

$$\tau^{s(m,k)eq} = \tau_F^{(m)} - \kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)})T, \quad (8)$$

where $\kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)})$ is an empirical function specifying the temperature dependence and $\tau_F^{(m)}$ may be a constant or a distributed quantity with some density $\psi^{(m)}(\tau^{(m)})$. To calculate the evolution of the deformation hardening component of the flow stress $\tau^{s(m,k)def}$ we assume that the hardening modulus $h^{(m)}$ depends linearly on the amount of shear on the plane so that its rate $\dot{\tau}^{s(m,k)def}$ is equal to $h^{(m)}\dot{\Gamma}_\beta^{(m,k)}$. Besides hardening there may take place some recovery processes which lead to the decrease of the flow stress with the rate which has an Arrhenius-type dependency on temperature and that of power-type on the flow stress itself. Thus

$$\dot{\tau}^{s(m,k)def} = h^{(m)}\dot{\Gamma}_\beta^{(m,k)} - q(T)(\tau^{s(m,k)def})^{m_{\tau^s}}, \quad (9)$$

where $q(T) = r^{(m)} \exp\left(-\frac{U_m}{k_B T}\right)$; U_m , m_{τ^s} are empirical constants, k_B is the Boltzmann constant.

From (4) we obtain that in the plastic state it holds:

$$T_\tau^{(m,k)} = \tau^{s(m)eq} + \tau^{s(m,k)def} + C_\tau \sum_{m,k} \tau^{s(m,k)def}. \quad (10)$$

Taking time derivative of (10), using (8) and (9) and neglecting with the latent hardening addition to the flow stress we obtain that in the plastic flow state

$$\dot{T}_\tau^{(m,k)} = \frac{\partial \tau^{s(m)eq}}{\partial T} \dot{T} + \frac{\partial \tau^{s(m)eq}}{\partial \dot{\Gamma}_\beta^{(m,k)}} \ddot{\Gamma}_\beta^{(m,k)} + h^{(m)}\dot{\Gamma}_\beta^{(m,k)} - q(T)(\tau^{s(m,k)def})^{m_{\tau^s}}, \quad (11)$$

or after some transformations

$$P(T, \dot{\Gamma}_\beta^{(m,k)})\ddot{\Gamma}_\beta^{(m,k)} + h^{(m)}\dot{\Gamma}_\beta^{(m,k)} = \dot{T}_\tau^{(m,k)} - \kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)})\dot{T} + q(T)(\tau^{s(m,k)def})^{m_{\tau^s}}. \quad (12)$$

For $P(T, \dot{\Gamma}_\beta^{(m,k)}) = P(T)$, $\kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)}) = \kappa^{(m)} = \text{const}$ equation (12) becomes:

$$P(T)\ddot{\Gamma}_\beta^{(m,k)} + h^{(m)}\dot{\Gamma}_\beta^{(m,k)} = \dot{T}_\tau^{(m,k)} - \dot{\tau}_0^{s(m,k)}, \quad (13)$$

where

$$\dot{\tau}_0^{s(m,k)} = \kappa^{(m)}\dot{T} - q(T)(\tau^{s(m,k)def})^{m_{\tau^s}}. \quad (13a)$$

Assuming moreover in (13) $P(T) = 0$, and using Heaviside's functions to formulate the flow condition (4) and the second flow condition of the growth of the difference $T_\tau^{(m,k)} - \tau_0^{s(m,k)}$, we arrive at the system of equations

$$\begin{cases} \dot{\Gamma}_\beta^{(m,k)} = (h^{(m)})^{-1} [\dot{T}_\tau^{(m,k)} - \dot{\tau}_0^{s(m,k)}] \\ \dot{\tau}^{s(m,k) def} = h^{(m)} \dot{\Gamma}_\beta^{(m,k)} - q(T) (\tau^{s(m,k) def})^{m_\tau} \end{cases} \quad (14)$$

which solution allows to find the rate of athermal plastic deformation produced by the action of a given slip system. The deformation of the whole grain we get by taking the sum (1), and the macroscopic plastic deformation — by neutralization on all the grains constituting the polycrystal:

$$\varepsilon^a = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} R_\omega \varepsilon_\omega^{gr a} R_\omega^{-1}, \quad (15)$$

where R_ω is the rotation matrix transforming the laboratory basis into the crystallographic one of the grain ω .

Results of modeling

The approach described above has been applied to model plastic deformation of austenitic titanium-nickel alloy. According to the investigations of plasticity properties of titanium nickelide monocrystals [23] dislocation slip occurs on the crystallographic planes of two types namely $\{110\}$ and $\{100\}$. To clear out the contribution of the number of active slip systems there have been carried out calculations of stress-strain diagrams of a polycrystal for the cases when only one or both of these system were active. Yield stress recovery processes have been neglected ($q(T) = 0$), yield limits and hardening moduli have been taken equal for both slip systems. Typical result is presented in fig.10.

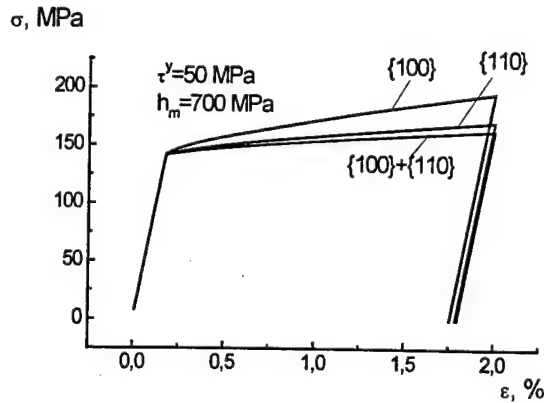


Fig.10. Calculated stress - strain diagrams of a model polycrystal, consisting of 20 grains when slip occurred on $\{100\}$, $\{110\}$ and both of these planes.

Variation of the hardening modulus and yield stress allowed to approximate different experimental curves. It may be concluded that polycrystal plastic properties do not depend strongly on the number and orientation of cristallographic slip planes. The situation is

different for monocrystals. Experimental data presented in the work [23] shows that both yield limits and hardening moduli strongly differ and are much bigger for a slip on $\{110\}$ planes. Rater good agreement with the experiment the present model shows whit the following values of parameters: for planes $\{100\}$ $\tau^{s\ eq} = 70$ MPa , $h^{(m)} = 800$ MPa and for planes $\{110\}$ $\tau^{s\ eq} = 320$ MPa , $h^{(m)} = 3000$ MPa (fig.11). At the same time there is no agreement when the tensile axis has an orientation $\langle 011 \rangle$ probably because of the anisotropy of the flow stress for different directions in the slip plane which was not accounted in this work.

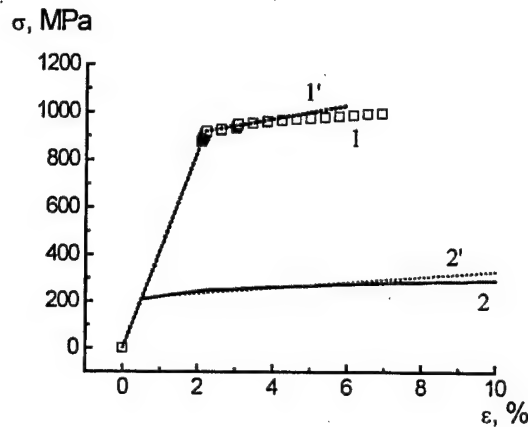


Fig.11 .Experimental (1,2) [23] and calculated (1',2') tensile diagrams of titanium nickelide monocrystals with the tensile axis oriented along $\langle 100 \rangle$ (curves 1,1') and $\langle 110 \rangle$ (curves 2,2')

Plastic deformation when produced in austenitic state of an SMA such as TiNi can be the cause of the reversible shape change when a specimen is thermocycled across the interval of the phase transformations. This phenomenon may be explained by the action of special intergranular stresses which appear in a polycrystal because of the plastic deformation anisotropy. An estimation calculation of the mean values of these stresses added to the approach described above shows a good qualitative agreement with the experiment (fig.12.). These results are soon to be published.

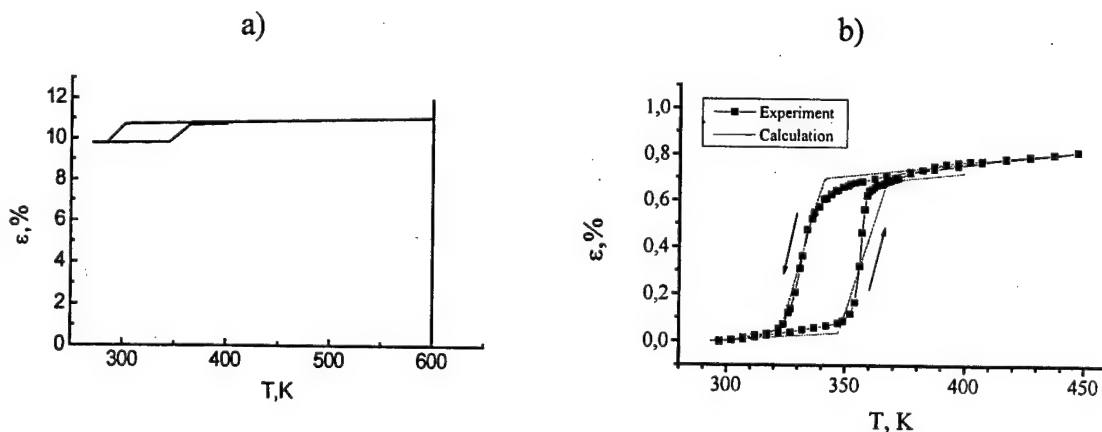


Fig.12 Strain variation at thermocycling of a TiNi specimen after an active plastic deformation at 600K:

a – calculation; b – fragment of fig.12a belonging under the transformation temperature interval compared with experimental data.

These results show that the structure-analytical model of strength outlined by V.A.Likhachev [9] is a good tool to describe the plastic behaviour of specific crystalline materials provided the mechanism of plasticity (slip planes, critical stresses, hardening moduli) are known. Particularly, the approach allows to model the deformation of shape memory alloys in different regimes of loading from the unique positions.

Experimental study of the influence of plastic strain on the shape memory effect of NiTi [2*]

The material utilized in this study was near equiatomic NiTi wires in both the as-received condition and after annealing at 850°C for 30 min. A differential scanning calorimeter (DSC) was used to determine the transformation temperatures and latent heat for the initial condition of the specimen. The mechanical loading portion of the test consisted of an isothermal tensile loading, at a temperature above austenite finish, that imparts a measurable plastic deformation into the specimen, as seen in the stress vs. strain curve of Fig.13. After loading, the specimen was heated in a stress free condition to separate the plastic strain from any stress-induced martensite that may have remained from the mechanical loading. This is followed by a thermal cycle, under a constant applied stress, resulting in a strain vs. temperature relationship, Fig.14, from which the phase transformation characteristics of start and finish transformation temperatures and transformation strain can be determined. The sequence of a mechanical loading followed by thermal loading was then repeated to observe a change in the phase transformation characteristics due to the increased level of plastic strain. This entire process was then repeated with the isothermal mechanical loading at a temperature below martensite finish. This was performed to distinguish between the effects of plasticity developed during phase transformation and plasticity developed during martensitic detwinning.

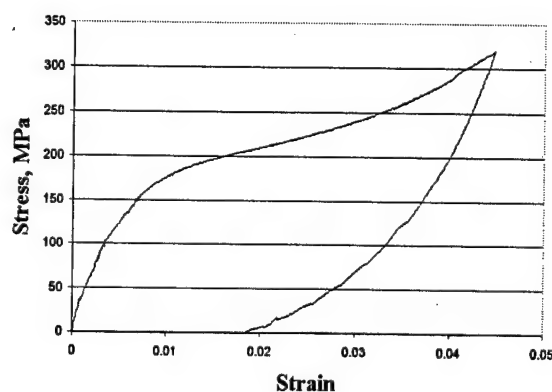


Fig.13 Stress vs. Strain for as-received SMA wire at $T > A_f$

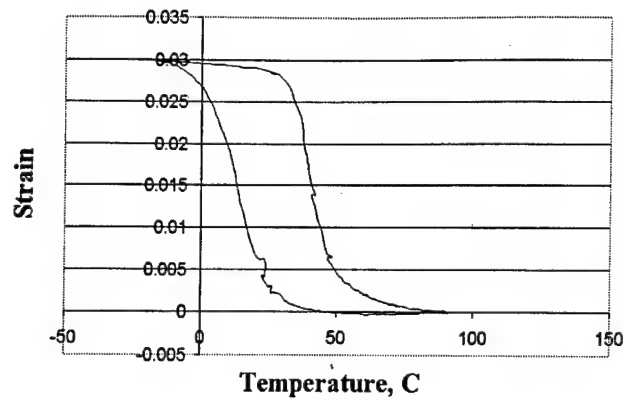


Fig.14 Strain vs. Temperature at 25 MPa after 9.0 % total plastic strain

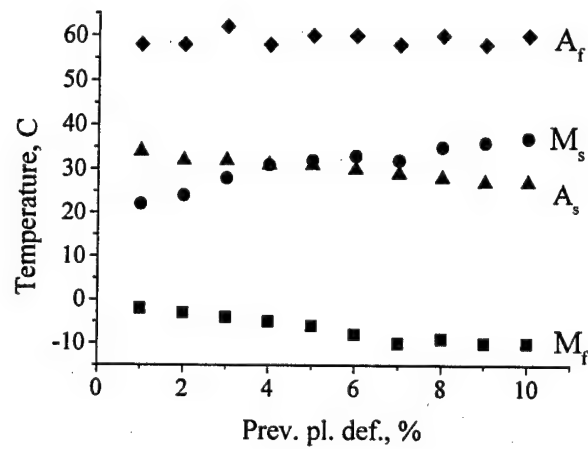


Fig.15 Dependence of phase transformation temperatures due to the previous plastic deformation.

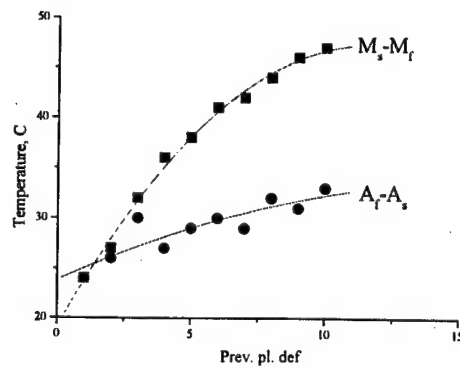


Fig.16 The transformation temperature start and finish differential due to the previous plastic deformation.

The following results represent a complete series of ten mechanical and subsequent thermal loadings at a temperature above austenite finish, A_f . Fig.15 demonstrates influence of plastic deformation on the characteristic temperatures of the phase transformation, measured from tests similar to Fig.14 for an as-received SMA wire. This data demonstrates that the plastic strain significantly effects the martensitic transformation temperatures and has a lesser impact on the austenitic transformation temperatures. Fig.16 quantifies the impact of the plastic strain on the transformation temperatures showing that differential between the martensitic start and finish temperatures grow at a rate more than double that of the austenitic start and finish temperatures.

References

- [1] T.W. Duerig, K.N. Melton, D. Stoeckel, C.M. Wayman, Engineering Aspects of Shape Memory Alloys, Butterworth-Heinemann, New York, 1990.
- [2] Shape Memory And Superelastic Technologies. Proceedings of the Second International Conference, 2-6 March 1997 Asilomar Conference Center, Pacific Grove, California, USA. Edited by Alan .Pelton, Darel Hodgson, Scott Russel and Tom Duerig. SMST. Sata Clara, California.,1997. 636 P.
- [3] Proceedings of the Second International Conference on Shape Memory and Superelastic Technologies (SMST-97), March 2-6, 1997, Asilomar Conference Center, Pacific Grove, California, USA, Ed. by A.R.Pelton, D.Hodgson, S.M.Russell and T.Duerig, 1997.
- [4] Bertram A. Thermomechanical constructive equations for the description of shape memory effect in alloys. Nucl. Engng. and Des. 1982. Vol. 74, N 2. P. 173-182.
- [5] Tanaka K., Iwasaki R. A phenomenological theory of transformation superplasticity. Engineering Fracture Mechanics. 1985. Vol. 21, N 4. P. 709-720.
- [6] Liang C., Rogers C. A. One-dimensional thermomechanical constitutive relations for shape memory materials. J. of Intelligent Materials Systems and Structures. 1990. Vol. 1, N 4, P. 207-234.
- [7] Lagoudas D. C., Bo Z., Qidwai M. A. A unified thermodynamic constitutive model for SMA and finite element analysis of active metal matrix composites. Mechanics of composite materials and structures. 1996. Vol. 3. P. 153-179.
- [8] F. Trochu, P. Terriault Nonlinear modeling of hysteresis material laws by dual kriging and application[3] Bertram
- [9] Likhachev V.A., Malinin V.G. Structure-analytical theory of strength. Saint-Petersburg, Nauka publ.h. , 1993. 471 P.(in Russian).
- [10] Likhachev V. A. Structure-analytical theory of martensitic unelasticity. J. Phys. Colloq. C.8, suppl. 1995. Vol. 5, N. 12. P. C8-137 - C8-142.
- [11] Volkov A.E., Evard M.E., Kurzeneva L.N., Likhachev V.A., Sakharov V.Yu., Ushakov V.V., "Mathematical modelling of martensitic inelasticity and shape memory effects", *Tech. Phys.* 41(11), 1084 - 1101 (1996).

- [12] Patoor E., Eberhardt A., Berveiller M. Micromechanical modelling of superelasticity in shape memory alloys. *Journal de Physique IV*, Coll. C1. 1996. Vol. 6. P. 277-292
- [13] Erglis I.V., Ermolaev V.A., Volkov A.E. A model of martensitic unelasticity accounting for the crystal symmetry of the material. *J.de Phys.*, Col. C8, Vol. 5, pp. 239 – 244.
- [14] Evard M.E., Volkov A.E. Modeling of martensite accommodation effect on mechanical behaviour of shape memory alloys. *J. of Engineering Materials and Technology*, 1999. - Vol.121.- P.102–104.
- [15] Patoor E., Siredey N., Eberhardt A., Berveiller M. Micromechanical approach of the fatigue behavior in a superelastic single cristal // *J. de Phys. IV*, 1995. Vol.5. P.C4 – 227 – 232.
- [16] Likhachev V.A., Kuzmin S.L., Kamentseva Z.P. Shape memory effect. Leningrad, LGU, 1987(in Russian).
- [17] Funakubo H. Shape Memory Alloys. Gordon & Breach, New York, 1987.
- [18] V.A. Likhachev, V.V. Rybin, O.G. Sokolov, S.L. Kuzmin, Transformation plasticity and mechanical memory at torsion in iron-manganese steels (in Russian), A.F.Ioffe OLFTI RAS (preprint 489), Leningrad, 1975. (in Russian).
- [19] L.A. Bizyukova, S.L. Kuzmin, V.A. Likhachev, "The phenomenon of strain recovery in Fe-Mn alloys", *Fizika metallov i metallovedenie*, 63 (3), 579–583 (1984).
- [20] M.E. Evard, A.E. Volkov, "Computer simulation of the shape memory effects in Fe-Mn type alloys accounting for the features of the fcc – hcp phase transformation", in *International Workshop on New Approaches to High-Tech Materials: Nondestructive Testing and Computer Simulations in Materials Science and Engineering*, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 3345, pp.178–183 (1998).
- [21] Belyaev S.P., Kuzmin S.L., Likhachev V.A., Kovalev S.M. Deformation and fracture of titanium nickelide under temperature cycles and stress. *Fizika Metallov i Metalloved.*, 1987 . Vol. 63, N 5, P.1017–1023 (in Russian).
- [22] Airoidi G., Ranucci T., Riva G., Sciacca A. The two-way memory effect in a 50 at. % Ti – 40 at. % Ni – 10 at. % Cu alloy // *J. Phys.: Condens. Matter*, 1995. Vol.7, N 19, P.3709 – 3720.
- [23] Chumlyakov YU.I, Surikova N.S., Korotaev A.D. Orientational dependence of strength and plasticity of titanium nickelide single crystals // *Fizika Metallov i Metalloved.*, 1996 . Vol. 82, N 7, P.148–158. (in Russian).

Modelling of martensite accommodation effect on mechanical behavior of shape memory alloys.

Evard M.E., Volkov A.E.

Res.Inst.Math.Mech.(NIIMM) of SPbSU, Bibliotechnaya pl., 2, Petrodvorets, 198904 St.-Petersburg, Russia

An approach has been presented to account for micro plastic deformation and stress produced by accommodation of martensite. This has made possible to describe such phenomena as incomplete recovery of strain, strain accumulation at thermocycling and repeated two-way shape memory effect. Results of modelling are in good qualitative agreement with experimental data.

Introduction

At present the structure-analytical theory of strength (Likhachev and Malinin, 1993) is successfully used to describe the mechanical behavior of alloys possessing the martensitic channel of non-elasticity. This theory postulates the deformation law on the microlevel, and the macro strain is calculated by neutralization of all micro strains related to the volumes with different crystallographic orientations and parameters of the transformation. Calculations have shown that this approach well describes the transformation plasticity, shape memory, pseudoelasticity and some other properties. However there has not been achieved a satisfactory description of shape memory alloys (SMA) behavior at cyclic temperature variations (the decrease of strain underrecovery with the number of cycles) and other properties, due to micro plastic strains produced at the growth of martensitic crystals, among them the repeated shape memory effect (Likhachev et al., 1987). The present work is an attempt to introduce into account this type of micro plasticity.

Model

The averaging procedure as in the work of Erglis et al., (1995) has been organized in a way to reflect the grain structure of the material. We have assumed that in each of $1, 2, \dots, \omega, \dots, \Omega$ grains of the polycrystalline object N crystallographically equivalent martensitic variants can appear. If the matrix D of the deformation due to the transformation by one of the variants is known, the corresponding matrices D_n for other variants can be found by rotating D by the operators P_n belonging to the cube symmetry group:

$$D_n = P_n D P_n^{-1}, \quad n = 1, \dots, N. \quad (1)$$

The volume fraction of martensite in a grain is equal to

$$\Phi^{gr} = \frac{1}{N} \sum_{n=1}^N \Phi_n, \quad (2)$$

For simplicity \hat{O}^{gr} , \hat{O}_n , ε^{gr} , etc here and further are written instead of $\hat{O}^{gr}(\omega)$, $\hat{O}_n(\omega)$, $\varepsilon^{gr}(\omega)$, etc. Here the quantity $(1/N)\hat{O}_n$ is the volume fraction of the n -th variant of martensite in the considered grain.

In each grain the average strain ε^{gr} accumulated in the course of the transformation related to the crystallographic basis is

$$\varepsilon^{gr} = \frac{1}{N} \sum_{n=1}^N \Phi_n D_n, \quad (3)$$

The macroscopic strain ε^m of the specimen due to the transformation we obtain by reducing matrices $\varepsilon^{gr}(\omega)$ to the laboratory basis and averaging on all the grains:

$$\varepsilon^m = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} R_{\omega} \varepsilon_{\omega}^{gr} R_{\omega}^{-1}, \quad (4)$$

where $R(\omega)$ is the rotation matrix transforming the laboratory basis into the basis of grain ω

To formulate the law of variation of \hat{O}_n we consider the thermodynamical equilibrium of the two-phase austenite-martensite system. We introduce the thermodynamic force F_n^t which is the difference of specific Gibbs energies of martensite and austenite. It can be split into thermal F_n^{th} and mechanical F_n^{mech} parts:

$$F_n^t = F_n^{tem} + F_n^{mech}, \quad F_n^{tem} = (T - T_0)(q_0/T_0), \quad F_n^{mech} = \tau \cdot D_n \quad (5)$$

Here T_0 is the temperature of the equilibrium of the two phases when there is no stress, q_0 is the latent heat ($q_0 < 0$), τ is the stress and \cdot denotes the contraction of tensors. Introducing the effective temperature $T_n^* = T + (T_0/q_0) \tau \cdot D_n$, we get the expression for F_n^t comprizing both thermal and mechanical components:

$$F_n^t = (T^* - T_0) \cdot (q_0/T_0). \quad (6)$$

It is generally assumed that a moving interface overcomes a resistance, due to the energy of martensite crystals nucleation and other barriers. We shall refer to the force responsible for the hysteresis as to the friction force F_n^{fr} and assume that it has a constant absolute value and opposes the movement of a phase boundary:

$$F_n^{fr} = |F^{fr}| \text{sign}(\dot{O}_n) \quad (7)$$

(we do not put minus sign in the right part of (7) because of the form in which equilibrium equation (9) will be written further). Besides F_n^{fr} , a resistance force F_n due to interphase stresses arises when a martensite crystal is growing. We postulate as the first approximation that this force is proportional to \dot{O}_n :

$$F_n = G_m \dot{O}_n, \quad (8)$$

where G_m is a constant. We note that, reflecting the kinetics of the transformation, equation (8) applies both to cases when martensite grows and when it shrinks. At the thermodynamic equilibrium there is the balance of forces:

$$F_n^t = F_n + F_n^{fr}. \quad (9)$$

When law (8) is specified constants $|F^{fr}|$ and G_m can be determined from the kinetics of the martensitic transformation when no stress is applied:

(a) at $T^* = M_s$ $\dot{O}_n = 0$ and from (6) — (9) we get $|F^{fr}| = (-q_0) \cdot (A_f - M_s) / (A_f + M_s)$;

(b) at $T^* = M_f$ $\dot{O}_n = 1$ and from (8), (9) it follows that $G_m = (-q_0) \cdot 2(M_s - M_f) / (A_f + M_s)$.

If we accept for phase equilibrium temperature an estimation $T_0 = (A_f + M_s)/2$ then we may rewrite the last formulas as $|F^{fr}| = (-q_0) \cdot (A_f - M_s) / (2T_0)$, $G_m = (-q_0) \cdot (M_s - M_f) / T_0$.

Equation (3) one can consider as a decomposition of the strain ε^R relative to some generalized basis $\{D_n\}$ with components \dot{O}_n and which we therefore shall interpret as the measures of strain. As the micro plastic strain ε^{mp} caused by the accommodation of martensite is connected with the same martensite crystals as the phase strain, we postulate that ε^{mp} can be expressed in the form similar to (3).

$$\varepsilon^{mp} = \frac{1}{N} \sum_{n=1}^N \Phi_n^p D_n \quad (10)$$

where \dot{O}_n^p is the measure of the micro plastic strain produced at the accommodation of crystals, belonging to the n -th variant of martensite in a given grain.

As the accommodation leads to a partial relaxation of interphase stresses, we assume that the resistance force F_n decreases by the quantity $G_m \dot{O}_n^p$. So we must change equation (8) for resistance force to

$$F_n = G_m (\Phi_n - \dot{O}_n^p) \quad (11)$$

We note that after (11) has been accepted instead of (8) formulas (a) and (b) for $|F^{fr}|$ and G_m are no more valid as the kinetics of the transformation is different when martensite accommodation takes place.

To obtain an evolution for \dot{O}_n^p we assume that its variation $d\dot{O}_n^p$ is proportional to that of the quantity of martensite $d\dot{O}_n$ and it occurs when the force F_n exceeds some yield limit F_n^y :

$$d\dot{O}_n^p = k d\Phi_n H(|F_n| - F_n^y) H(dF_n \text{sign} F_n), \quad (12)$$

where H is the function of Heaviside, k is the coefficient characterizing hardening. If $k = 0$ there is no micro plasticity, if $k \rightarrow 1$ there is ideal micro plasticity without hardening. As the resistance force F_n grows (decreases) only at the growth (decrease) of martensite, which in its turn can occur only at the growth (decay) of the thermodynamic force F_n^t , we have $\text{sign}(dF_n) = \text{sign}(dF_n^t)$ and

$$H(dF_n \text{sign} F_n) = H(dF_n^t \text{sign} F_n). \quad (13)$$

Substituting (11) into (9), passing to differentials and using (12) and (13) we arrive at:

$$d\Phi_n = dF_n^t / \{G_m [1 - kH(|F_n| - F_n^y)H(dF_n^t \text{sign} F_n)]\} \quad (14)$$

Next we must take into account that micro plastic strain is accompanied by the hardening of material. To do this, as it is done in the classical theory of plasticity, we assume that the yield limit grows at the same rate as the resistance force which increment is equal to that of the thermodynamic force.

$$dF_n^y = dF_n^t H(|F_n| - F_n^y) H(dF_n^t \text{sign} F_n). \quad (15)$$

To get the initial conditions we use the fact that at temperatures above A_f and in stress-free state no micro deformations have begun and for all martensite variants we have $F_n^y = F_0^y = \text{const}$, $\dot{O}_n^p = \dot{O}_n = 0$.

When microplasticity is taken into account, the strain in a grain is calculated as

$$\varepsilon^{gr} = \frac{1}{N} \sum_{n=1}^N D_n (\Phi_n + \Phi_n^p), \quad (16)$$

and the total macro strain is delivered by averaging (4). Relations given above can be reduced to a system of $\Omega \cdot N$ ordinary differential equations, which have been used to model the behavior a specimen made of an alloy of TiNi type containing 120 grains of different pseudo-random orientations. The following values of material constants have been used: $M_f = 280$ K, $M_s = 300$ K, $A_s = 340$ K, $A_f = 360$ K, $T_0 = 330$ K, $q_0 = -150$ MJ/m³. The value $F_0^y = 13$ MPa has been chosen in such a way that microplasticity could take place at cooling of specimen stressed by 30 MPa. Parameter k has been varied. Calculations have been performed for cases of pure shear and uniaxial tension. Heat expansion has not been taken into account.

Modelling of cyclic loading

Microplastic deformation at accommodation of martensite strongly influences mechanical behavior of shape memory alloys and especially at cyclic variations of temperature or stress. Because of this we have chosen to model strain accumulation and recovery by a specimen loaded with a constant stress of 100 MPa and subjected to temperature cycles through the full interval of the phase transformation. Fig.1 presents the kinetics of this process for $k = 0.4$. Maximum strain saturates, strain unrecovered in a cycle decreases and the hysteresis loop stabilizes in approximately 20 cycles (Fig.2).

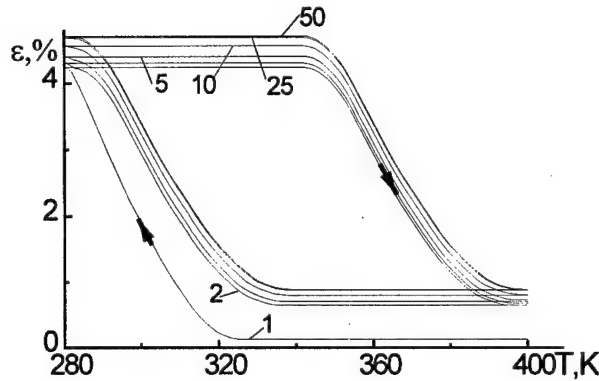


Fig.1 Strain vs. temperature dependence at thermocycling in the full interval of the martensitic transformation under the stress of 100 MPa. Numerals on the plot indicate numbers of cycles.

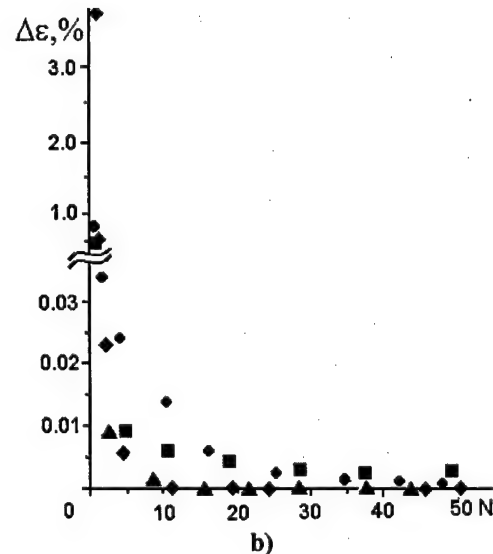
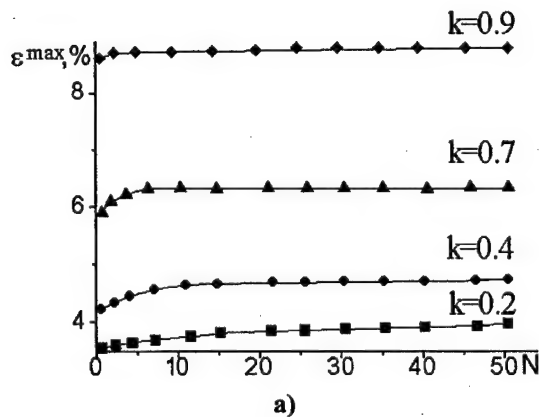


Fig.2. Calculated strain at a temperature below M_f (a) and the unrecovery of the strain (b) in an N -th cycle. Thermal cycling was carried out through the full interval of the martensitic transformation under the stress of 100 MPa symbols in fig.2b correspond to the values of k , given in fig.2a.

An important place in the studies of the work ability of SMAs is occupied by the following thermomechanical cycle: cooling of a sample from austenite to martensite under some load P , application of an additional load Q , heating to a temperature higher than A_f and removing the additional load Q to have the initial load P . Figures 3, 4 show the result of such numerical experiment when $P = 100$ MPa, $Q = 200$ MPa. Stabilization of the loop in this case is also achieved in about 20 cycles. Strain unrecovered in a cycle becomes small and almost constant. The maximum strain accumulated up to the N -th cycle slowly grows, these results are in a good agreement with the data of the direct experiment (Belyaev et al., 1987). An application of an additional load Q at a low temperature causes no unelastic strain as the stress produced by $P+Q$ is insufficient for the reorientation of martensite. As the temperature rises, the reorientation limit stress decreases. At some temperature lower than A_f the reorientation of martensite starts. Then a typical "hump" appears on the strain recovery curves in fig.3.

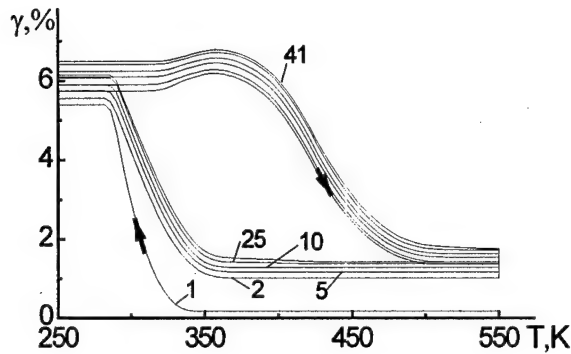
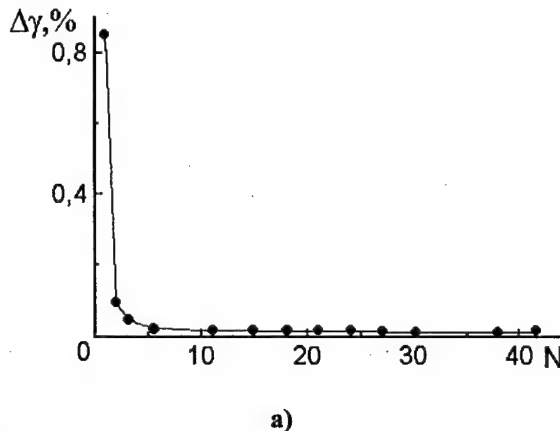
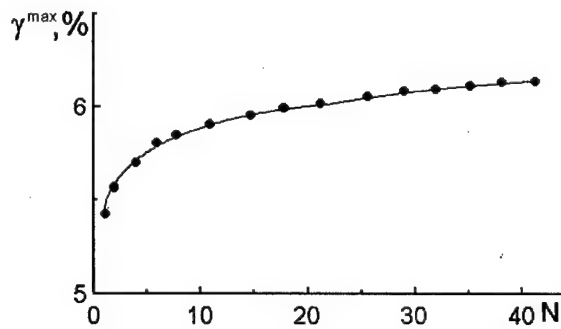


Fig. 3. Calculated strain versus temperature diagram at thermocycles with cooling under the stress 100 MPa and heating under 300 MPa (torsion). Numerals indicate numbers of cycles.



a)



b)

Fig. 4. Strain unrecovery (a) and maximum strain (b) as function of the number of thermocycles depicted in fig. 3.

Modelling of repeated two-way shape memory.

One of the properties of SMAs which until now could not be satisfactorily described in the scheme of the structure-analytical model is the repeated two-way shape memory (Likhachev et al., 1987) formed by cooling under a stress or by active straining in martensite. The mechanism of this phenomena may lie in the appearance of micro stress fields as the result of the incompatible plastic strain accompanying the growth of martensite crystals. Figures 5 and 6 present the results of modelling of this effect.

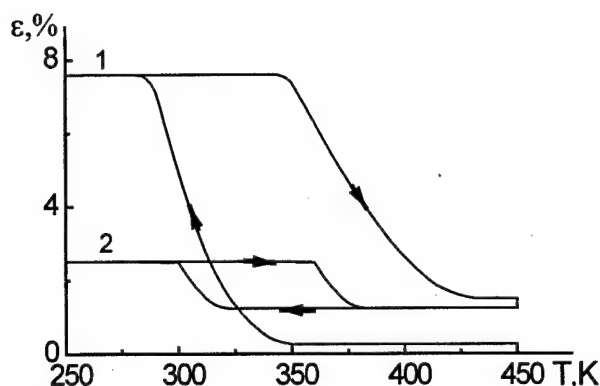


Fig. 5. Calculated strain versus temperature diagram at cooling and heating under 100 MPa (curve 1), unloading and a stress-free thermocycle (curve 2).

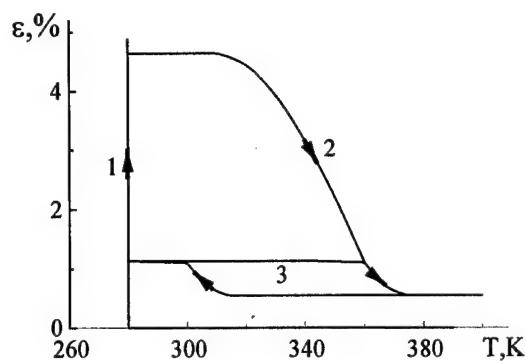


Fig. 6. Strain versus temperature diagram of active deformation of a sample in martensite state and unloading (curve 1), heating (curve 2) and subsequent stress-free thermocycle (curve 3).

The model demonstrates a reversible strain variation which corresponds to experimental data (Likhachev et al., 1987). According to existing notions (Kuzmin, 1980; Funakubo et al., 1987) plastic deformation at martensite accommodation plays an important role in training of the material by thermocycling under a load, fatigue damages, formation of eigenstresses responsible for adaptation of the material and formation of the repeated two-way shape memory. The last thesis is confirmed by the fact that the repeated shape memory appears only after a strong enough straining of the object by a load exceeding a critical level when there is no complete strain recovery.

At the same time all the previous considerations were mostly pure qualitative and did not allow a passage to engineering calculations. The proposed model sets a formal ground for such notions and the agreement of calculated results with experimental ones confirms the validity of this approach. As the result it became possible to model thermocyclic training and repeated two-way shape memory. Calibration of the material constants allows to obtain valid results for specific alloys.

Acknowledgements.

The authors are grateful to S.P.Belyaev for useful discussion.

The present work has been supported by the European Research Office of the US Army, project N 68171-97-M-5779, scientific supervisor Dr. R.Reichenbach.

This manuscript has not been published or been submitted for publishing anywhere.

References.

- Belyaev S.P., Kuzmin S.L., Likhachev V.A., Kovalev S.M. Deformation and fracture of titanium nickelide under temperature cycles and stress. *Fizika Metallov i Metalloved.*, 1987. Vol. 63, N 5, P.1017-1023 (in Russian).
- Erglis I.V., Ermolayev V.A., Volkov A.E. A model of martensitic unelasticity accounting for the crystal symmetry of the material // *J. de Phys.*, Col. C8, 1995. V.5. P.239-244.
- Funakubo H. *Shape Memory Alloys*. Gordon & Breach, New York, 1987.
- Kuzmin S.L. *Shape memory and transformation plasticity in metals*. Candidate of Sciences Dissertation, Leningrad, 1980.
- Likhachev V.A., Kuzmin S.L., Kamentseva Z.P. *Shape memory effect*. Leningrad, LGU, 1987 (in Russian).
- Likhachev V.A., Malinin V.G. *Structure-analytical theory of strength*. Saint-Petersburg, Nauka, 1993 (in Russian).

Modelling of strain accumulation and recovery due to fcc-hcp transformation at thermocycles

Margarita E. Evard, Alexandre E. Volkov

*Research Institute of Mathematics and Mechanics (NIIMM) of Saint-Petersburg State University,
Bibliotechnaya pl., 2 Petrodvorets, 198904, St.-Petersburg, Russia*

ABSTRACT

An account of crystallographic features of fcc \leftrightarrow hcp transformations as well as of plastic accommodation of martensite has allowed to describe accumulation of strain under a constant stress at cyclic variations of temperature. The model also gives the recovery of this strain at subsequent thermal cycles when the stress is removed.

Keywords: FeMn, martensitic transformation, modelling, plastic accommodation, plasticity, thermocycles, shape memory effect, unelastic strain.

1. INTRODUCTION.

One of the specific features of fcc \leftrightarrow hcp transformations is the multi-variance of both direct and reverse transformations^{1,2}. The result of it is that specimens loaded by a constant stress experience deformation when they undergo either of the transformations. Thus, considerable strain can be accumulated at thermal cycles. Large part of this strain is reversible and can be recovered at further cycles after the stress is removed¹. This fact suggests that the strain is due to transformations rather than to dislocation movement. Strain accumulation at thermocycles can be described by the structure-analytical theory of strength^{3,4} which is distinguished by two ideas: (1) the existence of limits of the size of growing martensite crystals and (2) the possibility that the strain has undergone at the direct transformation. The model based on only these two features predicts absolutely symmetrical behavior of a loaded sample in heating and in cooling. An attempt to account for an asymmetry has been made in⁵. However, approaches^{4,5} did not take into account microplastic strain arising at the growth of martensite crystals and leading to a partial accommodation of martensite and relaxation of interphase stresses. Because of this drawback the stabilization of the deformation of the model material occurs in 3 – 5 cycles rather than in several dozens as in an actual experiment. Strain recovery at thermal cycles without stress can not be described either. The way to account for microplastic deformation in alloys with transformations of TiNi type has been suggested in⁶. In the present work an attempt has been made to apply this methodology to alloys with fcc \leftrightarrow hcp transformations. Results of simulation of their mechanical behavior at thermal cycles obtained by the mentioned models are shown.

2. MODEL WITH MARTENSITE CRYSTAL SIZE LIMITATIONS

In consistence with the ideas (1) and (2) the equation determining the evolution of the amount of martensite Φ_n ($n=1, \dots, N$) belonging to any of the orientation variants of lattice deformation D_n should be written in the form

$$\begin{aligned} \dot{\Phi}_n = & -\frac{\dot{T}_n^*}{M_s - M_f} H(-\dot{T}_n^*) H(1 - \Phi_M) H(\Phi^0 - \Phi_n) H[M_s - \Phi_n(M_s - M_f) - T_n^*] - \\ & -\frac{\dot{T}_n^*}{A_s - A_f} H(\dot{T}_n^*) H(\Phi_M) H(\Phi_n - \Phi^H) H[T_n^* - \Phi_n(A_s - A_f) - A_f], \end{aligned} \quad (1)$$

the first term answers for the direct and the second for the reverse transformation. $T_n^* = T + (T_0 / q_0) (\tau : D_n)$ is the effective temperature for the n -th variant; M_s , M_f , A_f , A_s are the characteristic temperatures of martensitic reactions; H is the Heaviside's function ($H(0)=1$); $\Phi_M = (1/N) \sum \Phi_n$ is the volume fraction of martensite obtained by averaging on all variants; dot denotes time derivative; τ is the stress tensor and q_0 (normally negative) is the latent heat of the transformation. Multiplicands $H(\Phi^0 - \Phi_n)$ and $H(\Phi_n - \Phi^H)$ show that direct and reverse transformations respectively are forbidden when the amount of martensite of the n -th variant is greater than Φ^0 or smaller than Φ^H . To reflect the second idea we put $\Phi^H < 0$ allowing negative values for Φ_n meaning that amount of austenite recovered from martensite by deformation — D_n exceeds the amount of martensite previously ob-

tained by deformation. In this model N is the number of all variants in all the grains. Macro strain is obtained by averaging:

$$\varepsilon = (1/N) \sum \Phi_n D_n. \quad (2)$$

Here integral should be used for continuous distribution of variants orientations. According to ⁶ satisfactory results are obtained with $\Phi^0=5$, $\Phi^H=-4$. Besides in ⁴ it has been shown that a better agreement with experiments can be obtained when the statistic scatter of such parameters as the strain temperature hysteresis width and its center are taken into account. For modelling we took the following values of material parameters: $\Phi^0=5$, $\Phi^H=-4$, $q_0=-63$ MJ/m³, $D_{31}=D_{13}=0,075$ (all the rest $D_{ik}=0$), $M_f=320$ K, $M_s=370$ K, $A_s=470$ K, $A_f=520$ K. Maximum deviations of the hysteresis width and center from their mean values were taken 75 K and 50 K respectively. All calculations were made for uniaxial tension. Elastic and heat expansion strains were not added. Typical diagrams of strain accumulation in a specimen at thermocycles across the interval 200 K – 620 K are shown in fig.1. Strain grows both at the direct and reverse transformations, its amount accumulated in one cycle decreases. Number of cycles to stabilize the strain was the same for simulations shown in figs. 1a and 1b, more cycles needed for bigger values of stress (fig.2).

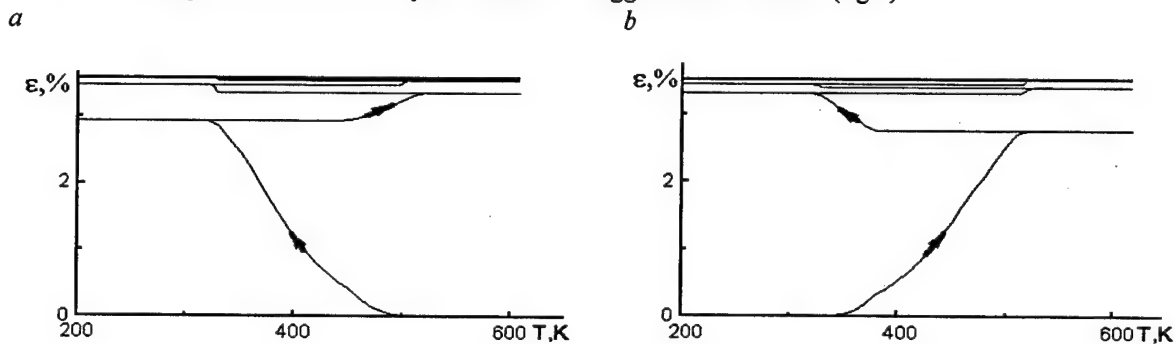


Fig.1. Dependencies of strain in the model object under a dead load 150 MPa on temperature at thermal cycles between 200 K and 600 K with initial state in austenite (a) or martensite (b).

These results qualitatively agree with direct observations of iron-manganese alloys ². In an actual experiments more cycles are needed to reach stabilization. Besides, calculations have shown that temperature M_s measured at the start of straining decreases (fig.3), this fact often explained entirely by the growth of the dislocation density ⁷.

Thus this approach has demonstrated the possibility of a satisfactory simulation of deformation at temperature variations. We note that only strain due to transformations was taken into account.

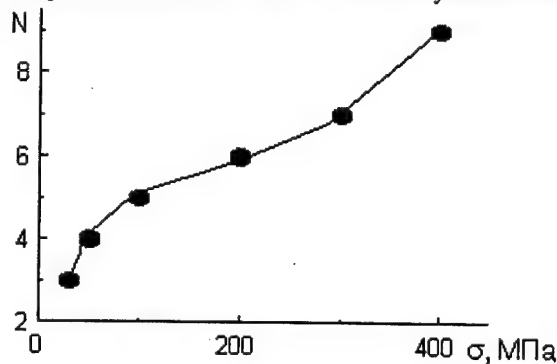


Fig.2. Dependence of the number of cycles to strain stabilization on stress at thermocycling across the interval of the transformation.

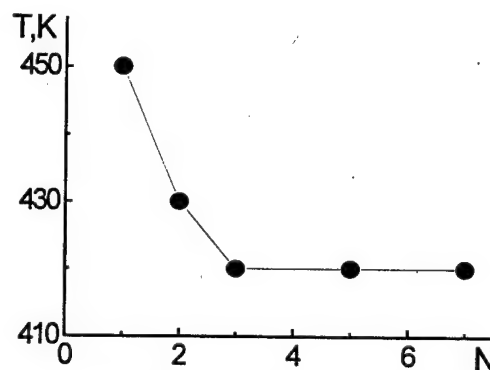


Fig.3. Temperature of the start of straining versus number of thermal cycles under a constant stress 150 MPa.

3. MODEL INCLUDING MICROPLASTIC DEFORMATION

At $\text{fcc} \rightarrow \text{hcp}$ transformation one of $\{111\}_{\text{fcc}}$ planes becomes $(0001)_{\text{hcp}}$ by one of three shears $1/6 \langle 11\bar{2} \rangle_{\text{fcc}}$ on each second plane making up $N=12$ variants of transformation strain tensor D_n and martensite quantities Φ_n .

At the reverse transformation each of three shears $1/3 \langle 11\bar{2} \rangle_{\text{hcp}}$ restores the initial orientation of austenite. Thus all variants can be divided into four triplets (zones) with parameters

$$\Phi_z = \frac{1}{3} \sum_{n=3z-2}^{3z} \Phi_n, \quad z=1, 2, 3, 4, \quad (3)$$

characterizing the amount of martensite belonging to a zone, $(1/4) \Phi_z$ being the volume fraction of martensite of this zone. Parameters Φ_n themselves do not have physical meaning of martensite amounts as deformations D_n belonging to one zone produce martensite of the same orientation. Still Φ_n play the role of measures of the phase deformation.

As it was mentioned above an incorporation into the model of microplastic strain caused by accommodation of martensite is necessary to reach a quantitatively correct modelling of cyclic dependencies. We postulate that microplastic strain can be presented in a form similar to the lattice transformation strain and introduce measures of this strain Φ_n^p so that the total micro strain β in a grain is given by the formula

$$\beta = \frac{1}{N} \sum_{n=1}^N (\Phi_n + \Phi_n^p) D_n \quad (4)$$

To formulate the kinetics law for Φ_n we introduce the thermodynamic driving force

$$F_n^t = (T^* - T_0)(q_0 / T_0). \quad (5)$$

which is equal to the Gibbs potential change at the transformation of a unit volume of austenite into martensite of the n -th variant. When transformation is in process a moving interface experiences a resistance because of energy barriers of martensite crystals nucleation and other obstacles. The corresponding force responsible for the existence of the hysteresis we settle to call the friction force F_n^{fr} and assume that it has a constant absolute value and hinders the transformation:

$$F_n^{fr} = -|F_n^{fr}| \text{sign}(\Delta \Phi_n) \quad (6)$$

Another opposing force F_n is that due to the appearance of interphase stresses. It grows with Φ_n and is relaxed by microplastic deformation Φ_n^p . Thus we assume:

$$F_n = G_m (\Phi_n - \Phi_n^p) \quad (7)$$

G_m is a material parameter. In terms of these forces thermodynamic equilibrium equation is

$$F_n^t = F_n^{fr} + F_n. \quad (8)$$

which we used to determine the conditions allowing the transformation.

Evolution equation for Φ_n^p we take in the form analogous to that in the classical theory of plasticity where driving thermodynamic force stands for the stress. Microplastic flow occurs when force F_n exceeds a yield limit F_n^y and $|F_n|$ continues to grow. Thus, when $H(|F_n| - F_n^y) H(dF_n \text{sign} F_n) > 0$ we postulate

$$d\Phi_n = (1/h_m) dF_n \quad (9)$$

with some module of microplasticity. Combining (7) and (9) we obtain an evolution equation for Φ_n when microplastic flow is on:

$$d\Phi_n = \frac{G_m + h_m}{G_m h_m} dF_n H(|F_n| - F_n^y) H(dF_n \text{sign} F_n). \quad (10)$$

One must keep in mind that microplastic deformation may be accompanied by hardening. To account for this we assumed that the yield limit increment dF_n^y is proportional to $d\Phi_n^p$: $dF_n^y = h'_m d\Phi_n^p$ (h'_m is some extra material parameter). Prior to any plastic deformations $F_n^y = F_0^y = \text{const}$ for all variants of martensite.

In iron manganese alloys we have two extra conditions of transformation finish: direct transformation can not occur to make the volume fraction of martensite in a grain $\Phi_g^s > 1$; martensite fraction in a zone $(1/4) \Phi_z$ can not become less than zero. Summarizing all this we arrive at a final form of the evolution equation:

$$dF_n = \left\{ \frac{G_m + g_m}{G_m g_m} \left[H(|F_n| - F_n^y) H(-dF_n^t \text{sign} F_n) + H(F_n^y - |F_n|) \right] dF_n + \right. \\ \left. + \frac{G_m + h_m}{G_m h_m} H(|F_n| - F_n^y) H(dF_n^t \text{sign} F_n) dF_n \right\} H(1 - F_n^s) H(F_z), \quad (11)$$

For numerical simulations the initial value of the yield limit ($F_0^y = 10$ MPa) was chosen such that microplasticity in cooling (and subsequent unrecovered strain in heating) took place when the stress was as small as 10 MPa. The value of the microplasticity module h_m was varied; h'_m was taken equal to h_m . Fig.4 presents the calculated by this model (for $h_m = 2$ MPa) diagram of strain evolution at thermal cycles as in fig.1a, stabilization

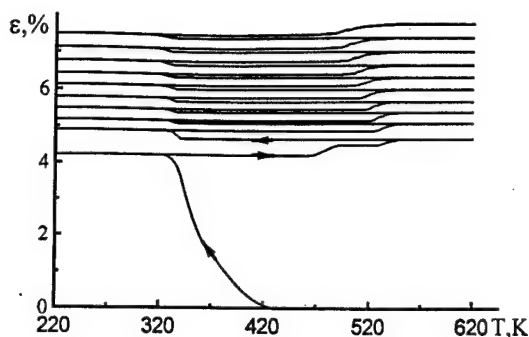


Fig. 4. Strain dependence on temperature at thermal cycles in the range 220 - 620 K under a constant stress of 50 MPa (calculation).

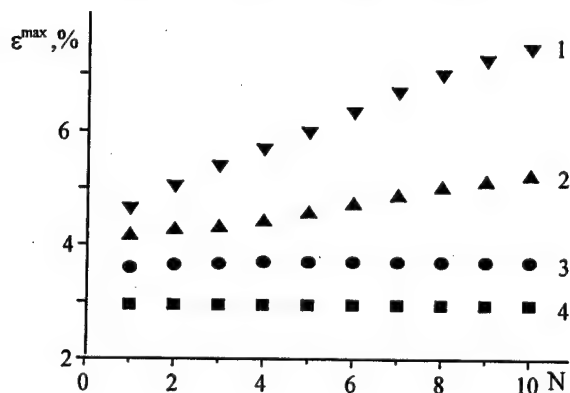


Fig. 5. Maximum strain accumulated by a model sample in N thermal cycles under stress 50 MPa for different values of module h_m : 2 (1), 5 (2), 7 (3), 65 (4) MPa.

of the strain being more gradual. By adjusting of module h_m one can obtain different rates of thermocyclic strain production (fig.5). The decrease of M_s observed at simulations is similar to that in fig.3

Appearance of microplastic strain gives rise to some of internal stress which is obviously the cause of the experimentally observed ⁸ partial strain recovery at subsequent thermal cycles in an unloaded specimen. Some confirmation to this statement is supplied by the result of modelling shown in fig.6. Very intensive in some first cycles the recovery in a cycle then decreases. In previous works this effect was not possible to describe by means of the structure-analytical model.

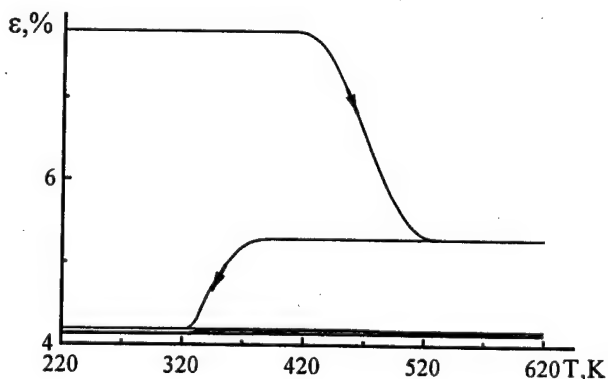


Fig. 6. Strain dependence on temperature at thermal cycles without stress after preliminary treatment shown in fig. 4.

In conclusion we may state that a satisfactory simulation of the cyclic mechanical behavior of alloys with $fcc \leftrightarrow hcp$ transformations is possible only with an account of the accommodation of martensite and microplastic deformation.

4. ACKNOWLEDGMENTS

This work has been carried out with the support of the European Research Office of the US Army, project N 68171-97-M-5779, scientific supervisor Dr. R. Reichenbach.

5. REFERENCES

1. V.A. Likhachev, S.L. Kuzmin, Z.P. Kamentseva, *Shape memory effect* (in Russian), LGU, Leningrad, 1987.
2. V.A. Likhachev, V.V. Rybin, O.G. Sokolov, S.L. Kuzmin, *Transformation plasticity and mechanical memory at torsion in iron-manganese steels* (in Russian), A.F. Ioffe OLFTI RAS (preprint 489), Leningrad, 1975.
3. V.A. Likhachev, V.G. Malinin, *Structure-analytical theory of strength* (in Russian), Nauka, Saint-Petersburg: 1993.
4. A.E. Volkov, M.E. Evard, L.N. Kurzeneva, V.A. Likhachev, V.Yu. Sakharov, V.V. Ushakov, "Mathematical modelling of martensitic inelasticity and shape memory effects", *Tech. Phys.* 41(11), 1084 – 1101 (1996).
5. M.E. Evard, A.E. Volkov, "Computer simulation of the shape memory effects in Fe-Mn type alloys accounting for the features of the fcc – hcp phase transformation", in *International Workshop on New Approaches to High-Tech Materials: Nondestructive Testing and Computer Simulations in Materials Science and Engineering*, Alexander I. Melker, Editor, Proceedings of SPIE Vol. 3345, pp.178–183 (1998).
6. M.E. Evard, A.E. Volkov, "Modelling of martensite accommodation effect on mechanical behavior of shape memory alloys", to be published in *Journal of Engineering Materials and Technology* (1998).
7. R. B. Perez-Saez, M. L. No, J. San Juan, "Influence of thermal cycling in a Fe-Mn-Si-Cr shape memory alloy", *J. de Phys. IV*, 5, C2–443–448 (1995).
8. L.A. Bizyukova, S.L. Kuzmin, V.A. Likhachev, "The phenomenon of strain recovery in Fe-Mn alloys", *Fizika metallov i metallovedenie*, 63 (3), 579–583 (1984).

A THEORETICAL STUDY OF THE PLASTIC DEFORMATION IN TITANIUM-NICKEL SHAPE MEMORY ALLOY

M.E.Evard and A.E.Volkov
Research Institute of Mathematics and Mechanics
of the Saint-Petersburg State University,
Bibliotechnaya pl.,2, Petrodvorets
198904 Saint-Petersburg Russia

Phone: 7-(812) 428-7079

Fax: 7-(812) 428-7039

E-mail: volkov@smel.math.spbu.ru and rita@smel.math.spbu.ru

ABSTRACT

Micromechanical modeling of the plastic deformation of austenitic titanium-nickel shape memory alloy poly- and monocrystals has been performed. The model assumes that the material consists of grains in which specific to this alloy slip systems become active when the shear stress reaches a critical value. The plastic flow goes on at stress the increase of which is determined by a hardening modulus. To find the parameters of the model existing experimental data on the plastic properties of monocrystals have been used. Calculated deformation diagrams of monocrystals with different orientations of the tensile axis show a good agreement with experiment.

INTRODUCTION

The behavior of shape memory alloys (SMAs) depends significantly on the internal structure of the material. In particular, plastic deformation shows influence on the quantitative characteristics and kinetics of martensitic non-elasticity, gives way to the formation of such specific effects as the two-way shape memory and training of the material at cyclic temperature variations (Likhachev, Kuzmin and Kamentzeva, 1987; Belyaev, Kuzmin, Likhachev and Kovalyev, 1987; Airoidi, Ranucci, Riva and Sciacca, 1995). Preliminary thermomechanical treatment allows to change purposefully the functional-mechanical properties of SMAs. That is why big attention is paid to the development of models allowing to calculate plastic deformation and predict its influence. Several works are devoted to the calculation of the dislocation plasticity arising at the growth of martensite crystals inside the austenitic matrix. It has been shown that accommodation processes are connected with such phenomena as the decrease of the phase yield limit at cyclic loading (Patoor, Siredey, Eberhardt and Berveiller, 1995), accumulation of irreversible strain at thermal cycling under a load or without it (Bo, Lagoudas, 1998; Evard, Volkov, 1999). The main principles of the calculation of the plastic deformation due to dislocation slip have been formulated in the book (Likhachev, Malinin, 1993). The present work is an attempt using the general ideas of this book to develop a model of the plastic deformation of polycrystalline TiNi specimen.

THEORETICAL MODEL

The mathematical object is an austenitic polycrystal consisting of grains numbered $1, 2, \dots, \omega, \dots, \Omega$, each grain having several slip systems. Any slip plane may be referred to one of $1, 2, \dots, m, \dots, M$ types and $1, 2, \dots, k, \dots, K_m$ crystallographically equivalent planes belong to each type. These planes may be obtained from one of them by rotations belonging to the point symmetry group of cubic lattice.

Athermal plastic deformation $\epsilon_{\omega}^{gr a}$ in a grain is the sum of the deformations on each of the slip planes in this grain:

$$\dot{\epsilon}_{\omega}^{gr a} = \sum_{m=1}^M \sum_{k=1}^{K_m} \dot{\epsilon}_{\omega}^{a(m,k)}, \quad (1)$$

where $\epsilon_{\omega}^{a(m,k)}$ is the referred to the laboratory basis athermal deformation produced by slip on the k -th plane of the m -th type.

Let σ^{gr} be the effective stress applied to a grain. Then the stress acting on the plane (m, k) has shear components which may be written as:

$$\tau_{31}^{(m,k)} = A_{p3}^{(m,k)} A_{q1}^{(m,k)} \sigma_{pq}^{gr}, \quad \tau_{32}^{(m,k)} = A_{p3}^{(m,k)} A_{q2}^{(m,k)} \sigma_{pq}^{gr}, \quad (2)$$

where A_{pq} is the rotation matrix transferring the crystallographic basis of the grain ω into the crystallographic basis of the (m, k) plane. We assume that dislocation slip starts when the intensity of the tangential stress on the slip plane

$$T_{\tau}^{(m,k)} = \sqrt{\frac{1}{2}((\tau_{31}^{(m,k)})^2 + (\tau_{32}^{(m,k)})^2)} \quad (3)$$

reaches its critical value $\tau^{s(m,k)}$:

$$T_{\tau}^{(m,k)} = \tau^{s(m,k)} \quad (4)$$

Due to the tangential stress

$$\tau_{\lambda\mu}^{(m,k)} = \tau_{31}^{(m,k)}(\delta_{\lambda 1}\delta_{\mu 3} + \delta_{\lambda 3}\delta_{\mu 1}) + \tau_{32}^{(m,k)}(\delta_{\lambda 2}\delta_{\mu 3} + \delta_{\lambda 3}\delta_{\mu 2}) \quad (5)$$

a shear strain is produced, having the components

$$\dot{\beta}_{31}^{a(m,k)} = \frac{1}{2}\dot{\Gamma}_{\beta}^{(m,k)} \frac{\tau_{31}}{T_{\tau}}, \quad \dot{\beta}_{32}^{a(m,k)} = \frac{1}{2}\dot{\Gamma}_{\beta}^{(m,k)} \frac{\tau_{32}}{T_{\tau}}, \quad (6)$$

where $\dot{\Gamma}_{\beta}^{(m,k)} = \sqrt{2\dot{\beta}_{pq}^{a(m,k)}\dot{\beta}_{pq}^{a(m,k)}}$ is the intensity of the shear strain rate tensor on the plane (m, k) .

We assume that the flow stress $\tau^{s(m,k)}$ is the sum of an equilibrium value $\tau^{s(m,k)eq}$, which is the same for all planes of the given m -th type, and additions responsible for the deformation $\tau^{s(m,k)def}$ and latent hardening:

$$\tau^{s(m,k)} = \tau^{s(m,k)eq} + \tau^{s(m,k)def} + C_{\tau} \sum_{m,k} \tau^{s(m,k)def}, \quad (7)$$

where C_{τ} is an empirical constant and the last term is due to the latent hardening connected with the possibility of simultaneous plastic deformation on several slip planes. This formula does not take into account the strain rate dependence of the flow stress.

The component $\tau^{s(m,k)eq}$ we shall write as follows:

$$\tau^{s(m,k)eq} = \tau_F^{(m)} - \kappa^{(m)}(T, \dot{\Gamma}_{\beta}^{(m,k)})T, \quad (8)$$

where $\kappa^{(m)}(T, \dot{\Gamma}_{\beta}^{(m,k)})$ is an empirical function specifying the temperature dependence and $\tau_F^{(m)}$ may be a constant or a distributed quantity with some density $\psi^{(m)}(\tau^{(m)})$.

To calculate the evolution of the deformation hardening component of the flow stress $\tau^{s(m,k)def}$ we assume that the hardening modulus $h^{(m)}$ depends linearly on the amount of shear on the plane so that its rate $\dot{\tau}^{s(m,k)def}$ is equal to $h^{(m)}\dot{\Gamma}_{\beta}^{(m,k)}$. Besides hardening there

may take place some recovery processes which lead to the decrease of the flow stress with the rate which has an Arrhenius-type dependency on temperature and that of power-type on the flow stress itself. Thus

$$\dot{\tau}^{s(m,k) def} = h^{(m)} \dot{\Gamma}_\beta^{(m,k)} - q(T)(\tau^{s(m,k) def})^{m_{\tau^s}}, \quad (9)$$

where $q(T) = r^{(m)} \exp\left(-\frac{U_m}{k_B T}\right)$; U_m , m_{τ^s} are empirical constants, k_B is the Boltzmann constant.

From (4) we obtain that in the plastic state it holds:

$$\dot{T}_\tau^{(m,k)} = \tau^{s(m) eq} + \tau^{s(m,k) def} + C_\tau \sum_{m,k} \tau^{s(m,k) def}. \quad (10)$$

Taking time derivative of (10), using (8) and (9) and neglecting the time derivative of the latent hardening addition to the flow stress we obtain that in the plastic flow state

$$\dot{T}_\tau^{(m,k)} = \frac{\partial \tau^{s(m) eq}}{\partial T} \dot{T} + \frac{\partial \tau^{s(m) eq}}{\partial \dot{\Gamma}_\beta^{(m,k)}} \ddot{\Gamma}_\beta^{(m,k)} + h^{(m)} \dot{\Gamma}_\beta^{(m,k)} - q(T)(\tau^{s(m,k) def})^{m_{\tau^s}}, \quad (11)$$

or after some transformations

$$P(T, \dot{\Gamma}_\beta^{(m,k)}) \ddot{\Gamma}_\beta^{(m,k)} + h^{(m)} \dot{\Gamma}_\beta^{(m,k)} = \dot{T}_\tau^{(m,k)} - \kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)}) \dot{T} + q(T)(\tau^{s(m,k) def})^{m_{\tau^s}}. \quad (12)$$

For $P(T, \dot{\Gamma}_\beta^{(m,k)}) = P(T)$, $\kappa^{(m)}(T, \dot{\Gamma}_\beta^{(m,k)}) = \kappa^{(m)} = \text{const}$ equation (12) becomes:

$$P(T) \ddot{\Gamma}_\beta^{(m,k)} + h^{(m)} \dot{\Gamma}_\beta^{(m,k)} = \dot{T}_\tau^{(m,k)} - \dot{\tau}_0^{s(m,k)}, \quad (13)$$

where

$$\dot{\tau}_0^{s(m,k)} = \kappa^{(m)} \dot{T} - q(T)(\tau^{s(m,k) def})^{m_{\tau^s}}. \quad (13a)$$

Assuming moreover in (13) $P(T) = 0$, and using Heaviside's functions to formulate the flow condition (4) and the second flow condition of the growth of the difference $T_\tau^{(m,k)} - \tau_0^{s(m,k)}$, we arrive to the system of equations

$$\begin{cases} \dot{\Gamma}_\beta^{(m,k)} = (h^{(m)})^{-1} [\dot{T}_\tau^{(m,k)} - \dot{\tau}_0^{s(m,k)}] \\ \dot{\tau}^{s(m,k) def} = h^{(m)} \dot{\Gamma}_\beta^{(m,k)} - q(T)(\tau^{s(m,k) def})^{m_{\tau^s}}, \end{cases} \quad (14)$$

which solution allows to find the rate of athermal plastic deformation produced by the action of a given slip system. The deformation of the whole grain we get by taking the sum (1), and the

macroscopic plastic deformation — by neutralization on all the grains constituting the polycrystal:

$$\varepsilon^a = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} R_{\omega} \varepsilon_{\omega}^{gr^a} R_{\omega}^{-1}, \quad (15)$$

where R_{ω} is the rotation matrix transforming the laboratory basis into the crystallographic one of the grain ω .

RESULTS OF MODELING

The approach described above has been applied to model plastic deformation of austenitic titanium-nickel alloy. According to the investigations of plasticity properties of titanium nickelide monocrystals (Chumlyakov, Surikova and Korotaev, 1996) dislocation slip occurs on the crystallographic planes of two types namely $\{110\}$ and $\{100\}$. To clear out the contribution of either of these slip systems there have been carried out calculations of stress-strain

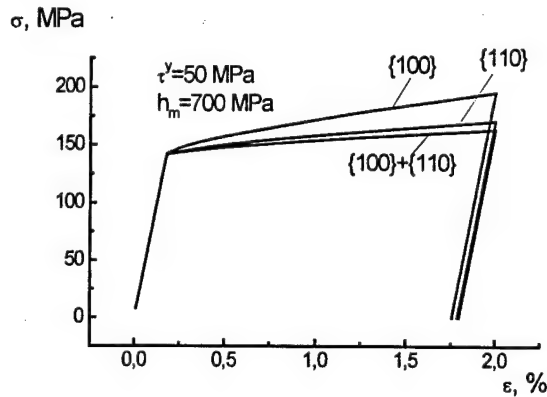


Fig.1. Calculated stress - strain diagrams of a model polycrystal, consisting of 20 grains when slip occurred on $\{100\}$, $\{110\}$ and both of these planes.

diagrams of a polycrystal for the cases when only one or both of these system were active. Yield stress recovery processes have been neglected ($q(T) = 0$), yield limits and hardening moduli have been taken equal for both slip systems. Typical result is presented in fig.1. Variation of the hardening modulus and yield stress allowed to approximate different experimental curves. It may be concluded that polycrystal plastic properties do not depend

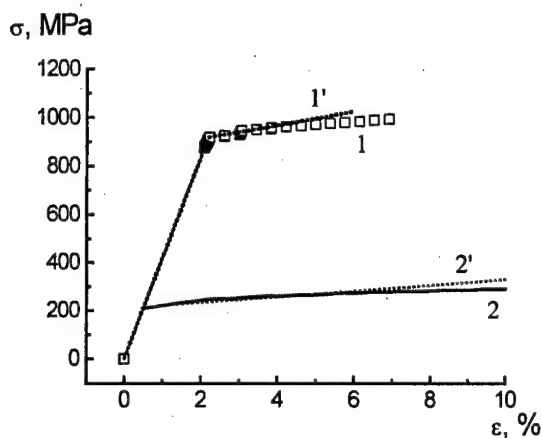


Fig.2 .Experimental (1,2) (Chumlyakov, Surikova and Korotaev,1996) and calculated (1',2') tensile diagrams of titanium nickelide monocrystals with the tensile axis oriented along $\langle 100 \rangle$ (curves 1,1') and $\langle 110 \rangle$ (curves 2,2')

strongly on the number and orientation of cristallographic slip planes. The situation is different for monocrystals. Experimental data presented in the work (Chumlyakov, Surikova and Korotaev,1996) shows that both yield limits and hardening moduli strongly differ and are much bigger for a slip on $\{110\}$ planes. Rater good agreement with the experiment the present model shows whit the following values of parameters: for planes $\{100\}$ $\tau^{s\ eq} = 70$ MPa , $h(m) = 800$ MPa and for planes $\{110\}$ $\tau^{s\ eq} = 320$ MPa , $h(m) = 3000$ MPa (fig.2). At the same time there is no agreement when the tensile axis has an orientation $\langle 011 \rangle$ probably because of the anisotropy of the flow stress for different directions in the slip plane which was not accounted in this work.

Making the resume of this work we may note that the structure-analytical model of strength outlined by V.A.Likhachev (Likhachev, Malinin,1993) is a good tool to describe the plastic behavior of specific crystalline materials provided the mechanism of plasticity (slip planes, critical stresses, hardening moduli) are known. Particularly, the approach allows to model the deformation of shape memory alloys in different regimes of loading from the unique positions.

ACKNOWLEDGEMENTS

The work has been carried out with the support of the European Research Office of the U.S. Army, project N 86171-97-M-5779, scientific supervisor Dr.R.Reichenbach.

REFERENCES

- AIROLDI G., RANUCCI T., RIVA G., SCIACCA A. The two-way memory effect in a 50 at. % Ti – 40 at. % Ni – 10 at. % Cu alloy // J. Phys.: Condens. Matter, 1995. Vol.7, N 19, P.3709 – 3720.
- BELYAEV S.P., KUZMIN S.L., LIKHACHEV V.A., KOVALEV S.M. Deformation and fracture of titanium nickelide under temperature cycles and stress. Fizika Metallov i Metalloved., 1987. Vol. 63, N 5, P.1017–1023 (in Russian).

- BO Z., LAGOUDAS D.C. // Accepted for publication in J.Eng.Sci., 1998.
- CHUMLYAKOV YU.I., SURIKOVA N.S., KOROTAEV A.D. Orientational dependence of strength and plasticity of titanium nickelide single crystals // Fizika Metallov i Metalloved., 1996. Vol. 82, N 7, P.148-158. (in Russian).
- EVARD M.E., VOLKOV A.E. Modelling of martensite accommodation effect on mechanical behavior of shape memory alloys // Journal of Engineering Materials and Technology, 1999, Vol. 121, N 1, p.102 - 104.
- LIKHACHEV V.A., KUZMIN S.L., KAMENTSEVA Z.P. Shape memory effect. Leningrad, LGU, 1987, 216 P. (in Russian).
- LIKHACHEV V.A., MALININ V.G. Structure-analytical theory of strength. Saint-Petersburg, Nauka, 1993 (in Russian).
- PATOOR E., SIREDEY N., EBERHARDT A., BERVEILLER M. Micromechanical approach of the fatigue behavior in a superelastic single crystal // J. de Phys. IV, 1995. Vol.5. P.C4 - 227 - 232.

INFLUENCE OF PLASTIC STRAIN ON THE SHAPE MEMORY EFFECT OF NiTi WIRES

David A. Miller¹, Dimitris C. Lagoudas¹
Margarite E. Evard² and Alexander E. Volkov²

¹Aerospace Engineering Department,
Texas A&M University
College Station, TX 77843-3141

²NIIMM St. Petersburg State University
Bibliotechnaja pl.2
198904 St. Petersburg, Russia

ABSTRACT: Fully annealed wires of NiTi are loaded mechanically under isothermal conditions until plastic deformation occurs. After unloading, a temperature cycle under a constant stress is applied to determine a relationship between the applied plastic strain and the phase transformation characteristics. Two sets of isothermal mechanical loadings are performed, with the first at a temperature below the martensitic finish temperature, and the second at a temperature above the austenitic finish temperature.

INTRODUCTION: Unlike common ductile metals, plastic deformation in shape memory alloys can be created by phase transformations and can occur at relatively low stress levels. Along with the creation of the plastic deformation, other material properties undergo significant changes with the accumulation of plastic strain. The austenite/martensite phase transformation characteristics of shape memory alloys have been shown in previous studies (Hebda and White [1995], Lim and McDowell, [1994], Liu and McCormick, [1990], McCormick and Liu, [1994], Perkins and Bobowiec [1986], Perkins and Sponholz [1984]) to be related to the loading history of the alloy. Both thermal cycles, mechanical cycles and cold working have shown an effect on the phase transformation thermomechanical properties such as start and finish temperatures, transformation strain and latent heat of transformation. The growth of plastic deformation has been successfully modeled and predicted by Bo and Lagoudas [1998] during thermally induced phase transformations under constant applied stress. To further develop and verify this model, experiments are conducted to study the influence of mechanically induced plastic deformation on the characteristics of the austenite/martensite phase transformation.

PROCEDURES, RESULTS AND DISCUSSION: The material utilized in this study was near equi-atomic NiTi wires in both the as-received condition and after annealing at 850°C for 30 min. A differential scanning calorimeter (DSC) was used to determine the transformation temperatures and latent heat for the initial condition of the specimen. The mechanical loading portion of the test consisted of an isothermal tensile loading, at a temperature above austenite finish, that imparts a measurable plastic deformation into the specimen, as seen in the stress vs. strain curve of Fig. 1. After loading, the specimen was heated in a stress free condition to separate the plastic strain from any stress-induced martensite that may have remained from the mechanical loading. This is followed by a thermal cycle, under a constant applied stress, resulting in a strain vs. temperature relationship, Fig. 2, from which the phase transformation characteristics of start and finish transformation temperatures and transformation strain can be determined. The sequence of a mechanical loading followed by thermal loading was then repeated to observe a change in the phase transformation characteristics due to the increased level of plastic strain. This entire process was then repeated with the isothermal mechanical loading at a temperature below martensite finish. This was performed to distinguish between the effects of plasticity developed during phase transformation and plasticity developed during martensitic detwinning.

The following results represent a complete series of ten mechanical and subsequent thermal loadings at a temperature above austenite finish, A_f . Fig. 3 demonstrates influence of plastic deformation on the characteristic temperatures of the phase transformation, measured from tests similar to Fig. 2 for an as-received SMA wire. This data demonstrates that the plastic strain significantly effects the martensitic transformation temperatures and has a lesser impact on the austenitic transformation temperatures. Fig. 4 quantifies the impact of the plastic strain on the transformation temperatures showing that differential between the martensitic start and finish temperatures grow at a rate more than double that of the austenitic start and finish temperatures.

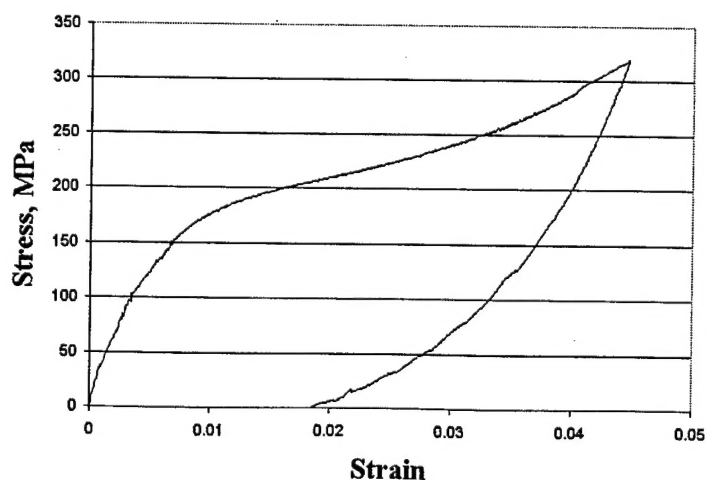


Figure 1 Stress vs. Strain for as-received SMA wire at $T > A_f$

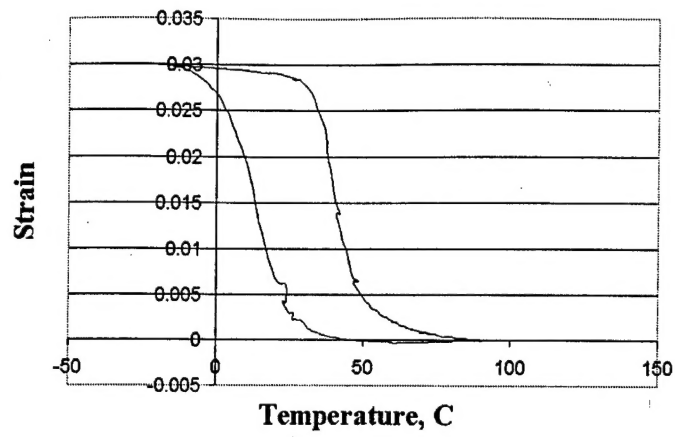


Figure 2 Strain vs. Temperature at 25 MPa after 9.0 % total plastic strain

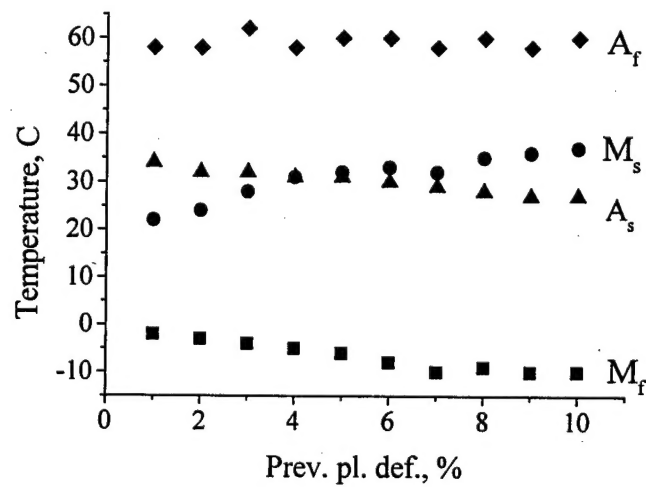


Figure 3 Dependence of phase transformation temperatures due to the previous plastic deformation.

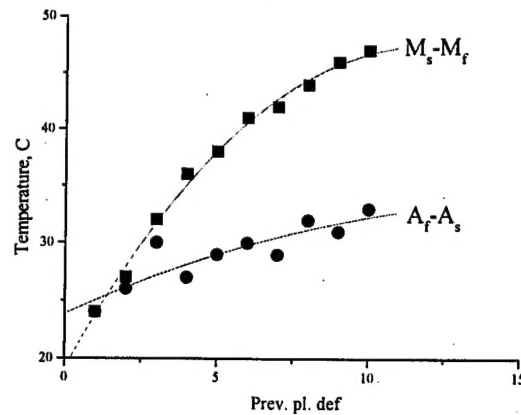


Figure 4 The transformation temperature start and finish differential due to the previous plastic deformation.

CONCLUSIONS: In this study, experiments were performed to identify the effect of plastic deformation on the phase transformation properties of NiTi. Test results show that the martensitic transformation temperatures widen as the plastic strain increases in the material. These results are consistent to those found for plastic strain development under cyclic thermal loading with constant applied stress.

ACKNOWLEDGEMENTS: The authors acknowledge the financial support of the Army Research Office.

REFERENCES:

- Bo, Z. and Lagoudas, D.C., 1998, Accepted for publication in Int J Eng Sci.
- Hebda, D. and White, S.R., 1995, Smart Materials and Structures}, Vol. 4, pp. 298-304.
- Lim, T.J., and McDowell, D.L., 1994, Proceedings of the 1994 North American Conference on Smart Structures and Materials, SPIE, Orlando, Florida, pp. 153-165.
- Liu, Y., and McCormick, P.G., 1990, Acta Metall. Mater, Vol. 38, No. 7, pp. 1321-1326.
- McCormick, P.G., and Liu, Y., 1994, Acta Metallurgica et Materialia, Vol. 42, No. 7, pp.2407-2413.
- Perkins, J and Sponholz, R.O., 1984, Metallurgical Transactions, Vol. 15A, pp. 313-321.
- Perkins, J. and Bobowiec, P., 1986, Metallurgical Transactions, Vol. 17A, No. 2, pp. 195-203.